

# Towards a Basis for Planar Two-Loop Integrals

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## Abstract

The existence of a finite basis of algebraically independent one-loop integrals has underpinned important developments in the computation of one-loop amplitudes in field theories and gauge theories in particular. We give an explicit construction reducing integrals with massless propagators to a finite basis for planar integrals at two loops, both to all orders in the dimensional regulator  $\epsilon$ , and also when all integrals are truncated to  $\mathcal{O}(\epsilon)$ . We show how to reorganize integration-by-parts equations to obtain elements of the first basis efficiently, and how to use Gram determinants to obtain additional linear relations reducing this all-orders basis to the second one. The techniques we present should apply to non-planar integrals, to integrals with massive propagators, and beyond two loops as well.

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## I. INTRODUCTION

The computation of higher-order corrections to amplitudes in gauge theories is important to the experimental program at particle colliders. Recent years have witnessed dramatic advances in technologies for computing one-loop amplitudes, critical to the program of next-to-leading order calculations for collider physics.

Important advances have also been made in computations of amplitudes beyond one loop. The computation of two-loop amplitudes relies in part on the ability to compute two-loop integrals, which has seen remarkable progress in the last decade. Several technologies [1] played a role in these advances, most notably the Mellin–Barnes approach to computing integrals pioneered by Smirnov [2] and Tausk [3], and later automated by Czakon [4]. Smirnov and Smirnov have recently introduced an alternative automated strategy for resolving singularities [5]. Anastasiou et al. have developed another method [6] of integral evaluation combining sector decomposition [7] with contour deformation [8]. These technologies have played a key role in higher-loop calculations in the  $\mathcal{N} = 4$  supersymmetric gauge theory [9, 10].

The computation of amplitudes has also made use of techniques for reducing arbitrary tensor integrals to a basis set of scalar *master integrals*. In calculations performed to date, the reductions have relied on integration by parts (IBP) [11] to construct linear equations relating the various integrals, and on Gaussian elimination in the form of the Laporta algorithm [12] to solve them. The solution determines a set of master integrals, and gives expressions for the remaining integrals in terms of them. This reduction approach has been automated in Anastasiou and Lazopoulos’s AIR program [13], in Smirnov’s FIRE program [14], and more recently, in Studerus’s **Reduze** program [15], as well as various private computer codes. We should note that the existence of a method, such as the Mellin–Barnes approach, for evaluating loop integrals directly means that a reduction to master integrals is not, strictly speaking, necessary for a Feynman-diagram calculation. It greatly reduces the complexity and difficulty of such calculations, however. In order to use master integrals in such calculations, one needs the explicit forms of the reduction equations.

Recent years have also witnessed the development and elaboration of a new set of technologies, so-called on-shell methods [16–22], for computing amplitudes. These rely only on knowledge gleaned from physical states. The unitarity method, one of the tools in this

approach, determines the rational coefficients of loop integrals in terms of products of tree amplitudes corresponding to cutting propagators in the loop amplitude. (These coefficients are rational in spinor variables.)

It is possible to determine the set of loop integrals that contribute to a given process during the computation of their coefficients, and most of the higher-loop computations to date have proceeded in this manner. In the most powerful form of the unitarity method, generalized unitarity [17, 23–25], one cuts an amplitude into more than two pieces; indeed, in ‘maximal unitarity,’ one cuts as many propagators as possible in a given contribution, thereby reducing any higher-loop amplitude to a product of basic tree amplitudes. The power of this technique is greatly enhanced by an *a priori* knowledge of a basis of integrals, as it then becomes possible to design the cuts in a general way.

Knowledge of a basis, in contrast, is essential to developing an automated numerical implementation, which several groups are currently pursuing at one loop [26]. The required basis has been known for a long time at one loop. The four-dimensional one dates back to the work of Melrose [27]. It is worth noting that the reduction equations themselves are not required when using generalized unitarity, because the method avoids the need for reductions of integrals with non-trivial numerators. We only need to know the set of algebraically independent master integrals. Baikov’s work [28] suggests an interesting connection between integration by parts and maximal unitarity.

Smirnov and Petukhov [29] have recently shown that the integral basis resulting from integration by parts is finite. In this paper, we give an explicit reduction to a finite set of integrals for planar integrals at two loops. There are two different kinds of bases we will consider. One requires algebraic independence to all orders in the dimensional regulator  $\epsilon$  (a “ $D$ -dimensional basis”), while the other requires algebraic independence for integrals truncated to  $\mathcal{O}(\epsilon^0)$  (a “regulated four-dimensional basis”). The latter contains fewer integrals, and is the relevant basis for the computation of amplitudes for numerical applications. We shall show how to limit the set of planar integrals that enter into a general two-loop computation, and discuss the reductions of some of these integrals. We leave the complete enumeration of basis integrals, as well as proofs of their algebraic independence, to future work.

The approach we will pursue here makes use of a chosen subset of IBP equations, designed to avoid the introduction of unwanted integrals with doubled propagators, as well as

supplementary Gram-determinant equations to take advantage of additional reductions possible when the loop integrals are performed in a truncated expansion about four dimensions rather than in arbitrary dimension (that is, to all orders in the  $\epsilon$  expansion). The approach we describe should also apply to non-planar integrals, and beyond two loops as well. We use the Mellin–Barnes approach [4, 5, 30, 31] to cross-check our equations, along with another technique for evaluating general higher-loop integrals, sector decomposition [7, 31].

We will not discuss the analytic evaluation of the master integrals. Integrals involving a single dimensionless ratio of invariants may be expressed in terms of harmonic polylogarithms introduced by Vermaseren and Remiddi [32], or alternatively in terms of the generalized polylogarithms of Goncharov [33]; some integrals involving two dimensionless ratios can be expressed in terms of a two-dimensional generalization of harmonic polylogarithms introduced by Gehrmann and Remiddi [34]; for examples, see ref. [35]. The four-mass double box was computed by Ussyukina and Davydychev [36, 37]. It is plausible that the complete set of two-loop basis integrals with massless internal lines can be expressed in terms of generalized polylogarithms, but this remains to be proven.

In section II, we review the basis of one-loop integrals with massless propagators in order to illustrate the two different bases, and to give a simple example of the use of Gram-determinant equations. In section III, we show how to reduce two-loop tensor and scalar integrals of sufficiently high multiplicity (again with massless propagators), thereby providing a constructive demonstration of the existence of a finite basis. We also describe how to obtain a compact set of equations relating only integrals relevant to amplitudes, avoiding the introduction of integrals with doubled propagators. In section V, we discuss the massless double box in detail. In section VI, we apply these techniques to double-box integrals with different patterns of external masses. In section VII, we apply the techniques to the pentabox integral. In section VIII, we give one example of the reduction of a six-point integral, the double pentagon. In section IX, we present a heuristic explanation of some of our results using generalized unitarity. We summarize in a concluding section.

## II. REDUCTION OF ONE-LOOP INTEGRALS

As a warm-up exercise, let us review integral bases at one loop along with their derivation. Throughout the paper, we will take the external momenta to be strictly four-dimensional.

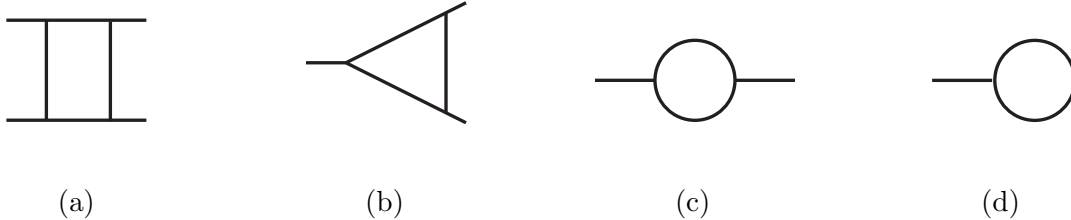


FIG. 1: The basis of scalar integrals: (a) box, (b) triangle, (c) bubble, and (d) tadpole. Each corner can have one or more external momenta emerging from it. The tadpole integral (d) vanishes when all internal propagators are massless.

They may be massless, or massive (representing, for example, sums of massless momenta in the original amplitude). In addition, we will take all vectors contracted with the loop momentum to be strictly four-dimensional as well. These vectors might be momenta or polarization vectors. All internal lines are taken to be massless.

In an  $n$ -point one-loop amplitude in gauge theory, we start with integrals with up to  $n$  external legs, and up to  $n$  powers of the loop momentum in the numerator. (In a gravitational theory, we would start with up to  $2n$  powers of the loop momentum. Up to questions regarding ultraviolet divergences, their treatment follows the same approach as the gauge-theory tensor integrals.) These powers are contracted with external momenta, external polarization vectors, or external currents. We shall denote the scalar integral by  $I_n$ ,

$$I_n(K_1, \dots, K_n) \equiv I_n[1] \equiv -i \int \frac{d^D \ell}{(2\pi)^D} \frac{1}{\ell^2(\ell - K_1)^2(\ell - K_{12})^2 \dots (\ell - K_{1\dots(n-1)})^2}. \quad (2.1)$$

In this equation,  $K_{j\dots l} = K_j + \dots + K_l$ . We denote integrals with a function of  $\ell$  inserted in the numerator as follows,

$$I_n[\mathcal{P}(\ell)] \equiv -i \int \frac{d^D \ell}{(2\pi)^D} \frac{\mathcal{P}(\ell)}{\ell^2(\ell - K_1)^2(\ell - K_{12})^2 \dots (\ell - K_{1\dots(n-1)})^2}, \quad (2.2)$$

where the momentum arguments are left implicit.

Let us begin with high-multiplicity integrals, with five or more external legs. Consider a

generic tensor integral<sup>1</sup>  $I_n[\ell \cdot v_1 \ell \cdot v_2 \cdots \ell \cdot v_n]$ . We shall make use of Gram determinants,

$$G\left(\begin{smallmatrix} p_1, \cdots, p_l \\ q_1, \cdots, q_l \end{smallmatrix}\right) \equiv \det_{i,j \in l \times l} (2p_i \cdot q_j), \quad (2.3)$$

$$G(p_1, \cdots, p_l) \equiv G\left(\begin{smallmatrix} p_1, \cdots, p_l \\ p_1, \cdots, p_l \end{smallmatrix}\right), \quad (2.4)$$

which have the useful property that they vanish if either the  $\{p_j\}$  or the  $\{q_j\}$  are linearly dependent. Using these objects, we can expand each of the four-dimensional vectors  $v_j$  in a basis of four chosen external momenta  $b_1, b_2, b_3, b_4$ ,

$$\begin{aligned} v^\mu = \frac{1}{G(b_1, b_2, b_3, b_4)} & \left[ G\left(\begin{smallmatrix} v, b_2, b_3, b_4 \\ b_1, b_2, b_3, b_4 \end{smallmatrix}\right) b_1^\mu + G\left(\begin{smallmatrix} b_1, v, b_3, b_4 \\ b_1, b_2, b_3, b_4 \end{smallmatrix}\right) b_2^\mu + G\left(\begin{smallmatrix} b_1, b_2, v, b_4 \\ b_1, b_2, b_3, b_4 \end{smallmatrix}\right) b_3^\mu \right. \\ & \left. + G\left(\begin{smallmatrix} b_1, b_2, b_3, v \\ b_1, b_2, b_3, b_4 \end{smallmatrix}\right) b_4^\mu \right]. \end{aligned} \quad (2.5)$$

This leads us to consider integrals with numerator insertions where all of the  $v_j$  are equal to one of the  $b_i$ . At one loop, these factors are all reducible, because we can rewrite any dot product as a difference of denominators, for example,

$$\ell \cdot b_1 = \frac{1}{2} [(\ell - K)^2 - (\ell - K - b_1)^2 + (K + b_1)^2 - K^2]. \quad (2.6)$$

The first two terms lead to integrals with fewer propagators and fewer powers of  $\ell$  in the numerator, while the last two lead to integrals with fewer powers of  $\ell$ ,

$$I_n[(\ell \cdot v)^n] \longrightarrow I_{n-1}[(\ell \cdot v)^{n-1}] \oplus I_n[(\ell \cdot v)^{n-1}]. \quad (2.7)$$

Repeating this procedure for the daughter integrals (with a new basis element instead of  $b_1$  where required) ultimately leads to integrals  $I_n$  with  $n \leq 4$  or with trivial numerators.

As is well known [27, 38–40], we can also reduce four- or fewer-point integrals with non-trivial numerators, by relying on Lorentz invariance to re-express them in terms of integrals where the non-trivial numerators involve only external momenta. (We could alternatively introduce additional basis vectors up to contributions from  $\mathcal{O}(\epsilon)$  numerators.) For the purposes of studying reductions, it therefore suffices to take  $v$  to be one of the external momenta even though the latter do not suffice to provide a basis. At higher loops, not all integrals can be reduced this way, because not all numerators can be written as differences of propagator

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<sup>1</sup> While this numerator does not have free indices, they could be exhibited by differentiating with respect to the  $v_j$ , so in a slight abuse of language, we will refer to the integral as a tensor integral.

denominators as in eq. (2.6). Many integrals with irreducible numerators can nonetheless be simplified using IBP technology as implemented (for example) in the Anastasiou–Lazopoulos AIR code [13] in Smirnov’s FIRE package [14], or in Studerus’s **Reduze** package [15], leaving a smaller set of master integrals.

We must next reduce the five- or higher-point integrals with trivial numerators (‘scalar’ integrals). While the reductions above hold independent of the dimensionality of the loop integration, the same is not true of all of the reductions we must consider here. We must distinguish between an integral basis to all orders in the dimensional regularization parameter  $\epsilon$ , and one which holds only through order  $\mathcal{O}(\epsilon^0)$ . The latter may contain fewer integrals than the former, because it is possible for linear combinations of integrals to be nonzero but of  $\mathcal{O}(\epsilon)$ . At one loop, this is indeed what happens, with the scalar pentagon integral required in an all-orders basis while being reducible to  $\mathcal{O}(\epsilon^0)$  [41].

Let first consider the reduction of six- or higher-point integrals, which can be done to all orders in  $\epsilon$ . Because the external momenta are four-dimensional, we have,

$$G\left(\begin{smallmatrix} \ell, 1, 2, 3, 4 \\ 5, 1, 2, 3, 4 \end{smallmatrix}\right) = 0, \quad (2.8)$$

where we have used the labels of the external momenta to represent the momenta themselves. Accordingly,

$$I_n\left[G\left(\begin{smallmatrix} \ell, 1, 2, 3, 4 \\ 5, 1, 2, 3, 4 \end{smallmatrix}\right)\right] = 0, \quad (n \geq 6). \quad (2.9)$$

If we now expand the Gram determinant,

$$\begin{aligned} G\left(\begin{smallmatrix} \ell, 1, 2, 3, 4 \\ 5, 1, 2, 3, 4 \end{smallmatrix}\right) &= -\ell^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 2, 3, 4 \end{smallmatrix}\right) + (\ell - K_1)^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, K_{12}, 3, 4 \end{smallmatrix}\right) \\ &\quad - (\ell - K_{12})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, K_{23}, 4 \end{smallmatrix}\right) + (\ell - K_{123})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, 2, K_{34} \end{smallmatrix}\right) \\ &\quad + (\ell - K_{1234})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, K_{45} \end{smallmatrix}\right) - (\ell - K_{12345})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, 4 \end{smallmatrix}\right) \\ &\quad - K_1^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, K_{12}, 3, 4 \end{smallmatrix}\right) + K_{12}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, K_{23}, 4 \end{smallmatrix}\right) \\ &\quad - K_{123}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, 2, K_{34} \end{smallmatrix}\right) - K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, K_{45} \end{smallmatrix}\right) \\ &\quad + K_{12345}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, 4 \end{smallmatrix}\right), \end{aligned} \quad (2.10)$$

we obtain an equation relating the  $n$ -point integral to six  $(n - 1)$ -point integrals,

$$I_n(K_1, \dots, K_n) = c_1 I_{n-1}(K_{n1}, K_2, \dots, K_{n-1}) + c_2 I_{n-1}(K_{12}, K_3, \dots, K_n)$$

$$\begin{aligned}
& + c_3 I_{n-1}(K_1, K_{23}, K_4, \dots, K_n) + c_4 I_{n-1}(K_1, K_2, K_{34}, K_5, \dots, K_n) \\
& + c_5 I_{n-1}(K_1, \dots, K_{45}, \dots, K_n) + c_6 I_{n-1}(K_1, \dots, K_{56}, \dots, K_n)
\end{aligned} \quad (2.11)$$

where

$$\begin{aligned}
c_0 &= -K_1^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, K_{12}, 3, 4 \end{smallmatrix}\right) + K_{12}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, K_{23}, 4 \end{smallmatrix}\right) - K_{123}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, 2, K_{34} \end{smallmatrix}\right) \\
&\quad - K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, K_{45} \end{smallmatrix}\right) + K_{12345}^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, 4 \end{smallmatrix}\right), \\
c_1 &= \frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 2, 3, 4 \end{smallmatrix}\right), \\
c_2 &= -\frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, K_{12}, 3, 4 \end{smallmatrix}\right), \\
c_3 &= \frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, K_{23}, 4 \end{smallmatrix}\right), \\
c_4 &= -\frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 5, 1, 2, K_{34} \end{smallmatrix}\right), \\
c_5 &= -\frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, K_{45} \end{smallmatrix}\right), \\
c_6 &= \frac{1}{c_0} G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, 4 \end{smallmatrix}\right).
\end{aligned} \quad (2.12)$$

One can check numerically that the coefficient  $c_0$  does not vanish for generic momenta, and hence the  $c_i$  are well-defined.

In  $D$  dimensions, as mentioned above, pentagon integrals are needed as independent basis elements. When expanding about  $D = 4 - 2\epsilon$  dimensions, however, only the  $\mathcal{O}(\epsilon)$  terms are independent, so that the integral can be eliminated from the basis. We can derive the required equation by considering the Gram determinant  $G(\ell, 1, 2, 3, 4)$ . The Gram determinant itself is of  $\mathcal{O}(\epsilon)$ , because it can avoid vanishing only when the  $\epsilon$  components of  $\ell$  appear in place of  $\ell$ . This leads us to consider the integral,

$$I_5[G(\ell, 1, 2, 3, 4)]. \quad (2.13)$$

One might worry that the Gram determinant can end up multiplying divergent terms in the integrand, yielding terms which are overall still of  $\mathcal{O}(\epsilon^0)$  or even divergent. However, all divergences of the integral arise from regions where  $\ell$  is soft, or collinear to one of the external legs. In these regions, the Gram determinant vanishes. Because the divergences are logarithmic at  $D = 4$ , any vanishing of the integrand suffices to eliminate the divergences. (At one loop, this in fact follows directly from the dependence of the integral only on the



$\epsilon$ -dimensional components of  $\ell$ ; but that will not necessarily be manifestly true for similar integrals we shall consider in the two-loop case.) Furthermore, the integral is ultraviolet-finite by power counting. Accordingly, the integral itself is also of  $\mathcal{O}(\epsilon)$ ,

$$I_5[G(\ell, 1, 2, 3, 4)] = \mathcal{O}(\epsilon). \quad (2.14)$$

We can use this to obtain a useful equation for the pentagon integral by expanding the Gram determinant, and re-expressing dot products of the loop momenta in terms of differences of denominators,

$$\begin{aligned} G(\ell, 1, 2, 3, 4) = & d_0 + d_1 \ell^2 + d_2 (\ell - K_1)^2 + d_3 (\ell - K_{12})^2 + d_4 (\ell - K_{123})^2 + d_5 (\ell - K_{1234})^2 \\ & - \ell^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ \ell, 2, 3, 4 \end{smallmatrix}\right) + (\ell - K_1)^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ \ell, K_{12}, 3, 4 \end{smallmatrix}\right) - (\ell - K_{12})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ \ell, 1, K_{23}, 4 \end{smallmatrix}\right) \\ & + (\ell - K_{123})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ \ell, 1, 2, K_{34} \end{smallmatrix}\right) - (\ell - K_{1234})^2 G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ \ell, 1, 2, 3 \end{smallmatrix}\right), \end{aligned} \quad (2.15)$$

where

$$\begin{aligned} d_0 = & -(K_1^2)^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ K_{12}, 3, 4 \end{smallmatrix}\right) + 2K_1^2 K_{12}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, K_{23}, 4 \end{smallmatrix}\right) - (K_{12}^2)^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, K_{23}, 4 \end{smallmatrix}\right) \\ & - 2K_1^2 K_{123}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) + 2K_{12}^2 K_{123}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) - (K_{123}^2)^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 1, 2, K_{34} \end{smallmatrix}\right) \\ & + 2K_1^2 K_{1234}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, 3 \end{smallmatrix}\right) - 2K_{12}^2 K_{1234}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, 3 \end{smallmatrix}\right) + 2K_{123}^2 K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 1, 2, 3 \end{smallmatrix}\right) \\ & - (K_{1234}^2)^2 G\left(\begin{smallmatrix} 1, 2, 3 \\ 1, 2, 3 \end{smallmatrix}\right), \\ d_1 = & 2G\left(\begin{smallmatrix} 1, 2, 3, 4 \\ 1, 2, 3, 4 \end{smallmatrix}\right) - K_1^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 2, 3, 4 \end{smallmatrix}\right) + K_{12}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 2, 3, 4 \end{smallmatrix}\right) - K_{123}^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 2, 3, 4 \end{smallmatrix}\right) \\ & + K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, 3 \\ 2, 3, 4 \end{smallmatrix}\right), \quad (2.16) \\ d_2 = & K_1^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ K_{12}, 3, 4 \end{smallmatrix}\right) - K_{12}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, K_{23}, 4 \end{smallmatrix}\right) + K_{123}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) - K_{1234}^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, 3 \end{smallmatrix}\right), \\ d_3 = & -K_1^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, K_{23}, 4 \end{smallmatrix}\right) + K_{12}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, K_{23}, 4 \end{smallmatrix}\right) - K_{123}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) + K_{1234}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, 3 \end{smallmatrix}\right), \\ d_4 = & K_1^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) - K_{12}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, K_{34} \end{smallmatrix}\right) + K_{123}^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 1, 2, K_{34} \end{smallmatrix}\right) - K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 1, 2, 3 \end{smallmatrix}\right), \\ d_5 = & -K_1^2 G\left(\begin{smallmatrix} K_{12}, 3, 4 \\ 1, 2, 3 \end{smallmatrix}\right) + K_{12}^2 G\left(\begin{smallmatrix} 1, K_{23}, 4 \\ 1, 2, 3 \end{smallmatrix}\right) - K_{123}^2 G\left(\begin{smallmatrix} 1, 2, K_{34} \\ 1, 2, 3 \end{smallmatrix}\right) + K_{1234}^2 G\left(\begin{smallmatrix} 1, 2, 3 \\ 1, 2, 3 \end{smallmatrix}\right). \end{aligned}$$

The integrals of the terms on the last two lines of eq. (2.15) will vanish, as they correspond to box integrals with  $\varepsilon(\ell, \dots)$  in the numerator. The integral of the  $d_0$  term is simply a pentagon, and the integrals of the  $d_{1,\dots,5}$  terms are box integrals. These reductions and relations yield the well-known basis shown in fig. 1.

Our aim is to extend these considerations to two-loop integrals. We will also introduce a new technique for reducing integrals with irreducible numerators to the set of master integrals, based on rewriting the system of IBP equations. We delineate the finite universal basis, while leaving a complete and detailed enumeration of it to future work.

### III. REDUCTION OF PLANAR TWO-LOOP INTEGRALS

#### A. The Integrals

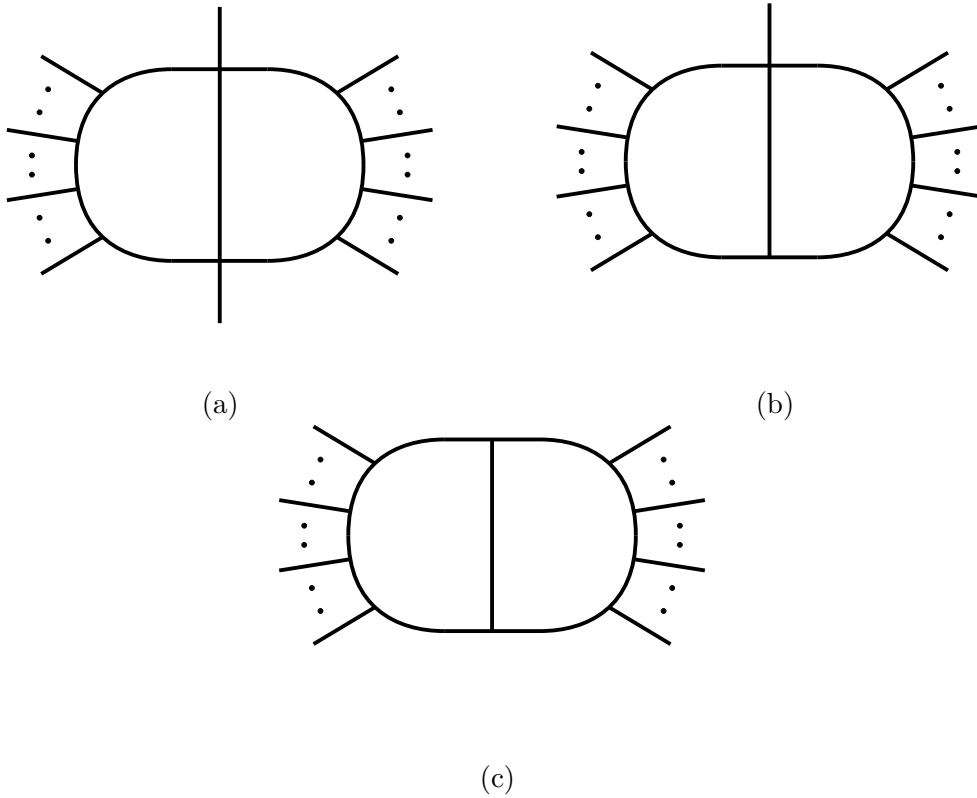


FIG. 2: The three basic types of two-loop planar integrals, labeled by the number of legs attached to each leg of the vacuum diagram: (a)  $P_{n_1, n_2}$ , (b)  $P_{n_1, n_2}^*$ , (c)  $P_{n_1, n_2}^{**}$ .

We turn now to our main object of study, the planar two-loop integrals. We can organize the different integral skeletons we obtain, representing only the propagators, into five classes. Three classes, depicted in fig. 2, arise from attaching external legs to the non-trivial two-loop vacuum diagram shown in fig. 3. We obtain planar integrals by attaching external legs to one or two of the internal lines, and possibly to its vertices. Were we to attach external legs to

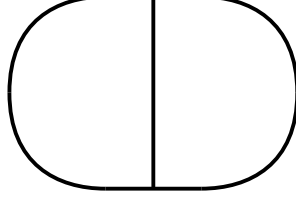


FIG. 3: The non-trivial two-loop vacuum diagram.

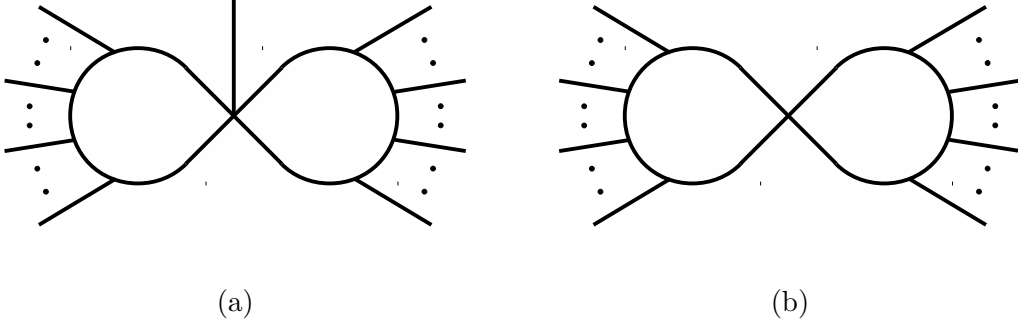


FIG. 4: Two-loop integrals which are products of one-loop integrals, labeled by the number of legs attached to each leg of the vacuum diagram: (a)  $I_{n_1, n_2}$ , (b)  $I_{n_1, n_2}^*$ .

the third internal line as well (here, the middle line), we would obtain non-planar integrals. This gives rise to three of the five types of two-loop planar integrals; the remaining types are simply products of one-loop integrals. We label the integrals according to the number of external legs attached to each of the vacuum diagram's internal lines, denoting the absence of lines attached to vertices by stars. The three types of integrals are,

$$\begin{aligned}
P_{n_1, n_2} &= (-i)^2 \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{1}{\ell_1^2 (\ell_1 - K_1)^2 \cdots (\ell_1 - K_{1 \dots n_1})^2 (\ell_1 + \ell_2 + K_{n_1 + n_2 + 2})^2} \\
&\quad \times \frac{1}{\ell_2^2 (\ell_2 - K_{n_1 + n_2 + 1})^2 \cdots (\ell_2 - K_{(n_1 + 2) \dots (n_1 + n_2 + 1)})^2}, \\
P_{n_1, n_2}^* &= (-i)^2 \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{1}{\ell_1^2 (\ell_1 - K_1)^2 \cdots (\ell_1 - K_{1 \dots n_1})^2 (\ell_1 + \ell_2)^2} \\
&\quad \times \frac{1}{\ell_2^2 (\ell_2 - K_{n_1 + n_2 + 1})^2 \cdots (\ell_2 - K_{(n_1 + 2) \dots (n_1 + n_2 + 1)})^2}, \\
P_{n_1, n_2}^{**} &= (-i)^2 \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{1}{\ell_1^2 (\ell_1 - K_1)^2 \cdots (\ell_1 - K_{1 \dots n_1})^2 (\ell_1 + \ell_2)^2} \\
&\quad \times \frac{1}{\ell_2^2 (\ell_2 - K_{n_1 + n_2})^2 \cdots (\ell_2 - K_{(n_1 + 1) \dots (n_1 + n_2)})^2},
\end{aligned} \tag{3.1}$$

along with products of two one-loop integrals shown in fig. 4,

$$I_{n_1, n_2} = (-i)^2 \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{1}{\ell_1^2 (\ell_1 - K_1)^2 \cdots (\ell_1 - K_{1 \dots n_1})^2}$$

$$\begin{aligned}
I_{n_1, n_2}^* &= (-i)^2 \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{1}{\ell_1^2 (\ell_1 - K_1)^2 \cdots (\ell_1 - K_{1 \dots n_1})^2} \\
&\quad \times \frac{1}{\ell_2^2 (\ell_2 - K_{n_1+n_2+1})^2 \cdots (\ell_2 - K_{(n_1+2) \dots (n_1+n_2+1)})^2}, \\
&\quad \times \frac{1}{\ell_2^2 (\ell_2 - K_{n_1+n_2})^2 \cdots (\ell_2 - K_{(n_1+1) \dots (n_1+n_2)})^2}, \tag{3.2}
\end{aligned}$$

so that  $P_{n_1, n_2}$  is an  $(n_1+n_2+2)$ -point integral,  $P_{n_1, n_2}^*$  and  $I_{n_1, n_2}$  are  $(n_1+n_2+1)$ -point integrals, and  $P_{n_1, n_2}^{**}$  and  $I_{n_1, n_2}^*$  are  $(n_1+n_2)$ -point integrals. Without loss of generality, we may take  $n_1 \geq n_2$ .

In our discussion below, we will focus on the  $P_{n_1, n_2}$  integrals. Similar arguments typically apply to the  $P_{n_1, n_2}^{*, **}$ . We may also observe that,

$$\begin{aligned}
P_{n_1, n_2}^*(K_1, \dots, K_{n_1+n_2+1}) &= P_{n_1, n_2}(K_1, \dots, K_{n_1+n_2+1}, 0), \\
P_{n_1, n_2}^{**}(K_1, \dots, K_{n_1+n_2}) &= P_{n_1, n_2}^*(K_1, \dots, K_{n_1}, 0, K_{n_1+1}, \dots, K_{n_1+n_2}). \tag{3.3}
\end{aligned}$$

so that the values of  $P^*$  and  $P^{**}$  are known in terms of  $P$ . Nonetheless, their different branch cut structures strongly suggest that the former are algebraically independent of the latter. In explicit examples in sections V–VIII, we examine  $P^{**}$  integrals.

These integrals will arise in the leading-color contributions to two-loop QCD amplitudes, including amplitudes for production of electroweak bosons or other particles coupled to quarks. Just as in the one-loop case, all internal lines will be massless, but the external legs of the integrals can correspond to sums of external momenta, and hence can be either massless or massive. Each of the vertices can come with a power of the corresponding loop momentum, and each of the three-point internal vertices in  $P_{n_1, n_2}^{*, **}$  can also come with a power of either  $\ell_1$  or  $\ell_2$ , so that we should consider tensor integrals with up to  $(n_1 + 2)$  powers of  $\ell_1$  along with  $n_2$  powers of  $\ell_2$ , or alternatively up to  $(n_1 + 1, n_2 + 1)$  or  $(n_1, n_2 + 2)$  powers of the two loop momenta  $(\ell_1, \ell_2)$ .

## B. Reduction of High-Multiplicity Integrals with Non-Trivial Numerators

We begin our discussion of integral reduction at two loops by considering tensor integrals with  $n_1 \geq 4$ ,  $P_{n_1, n_2}[\ell \cdot v_1 \ell \cdot v_2 \cdots \ell \cdot v_n]$ , where each  $\ell$  can be either  $\ell_1$  or  $\ell_2$ . We can use the expansion of eq. (2.5), with the external momenta  $b_1, \dots, b_4$  chosen amongst the first  $n_1$  momenta. This leads us to consider integrals with numerators containing factors of  $\ell_1 \cdot K_j$ ,

where  $1 \leq j \leq n_1$ . As in the one-loop case, these numerators are reducible,

$$\ell_1 \cdot K_j = \frac{1}{2}[(\ell_1 - K_{1\dots(j-1)})^2 - (\ell_1 - K_{1\dots j})^2 + K_{1\dots j}^2 - K_{1\dots(j-1)}^2]. \quad (3.4)$$

The first two terms lead to integrals with smaller indices ( $P_{n_1-1, n_2}$ ,  $P_{n_1-1, n_2}^*$ , or one of  $P_{n_1, n_1-1}$  and  $P_{n_1, n_1-1}^*$  in the case  $n_1 = n_2$ ) and simpler tensors, while the last two lead to integrals with simpler tensors. Repeating this procedure, including application to  $\ell_2$ , leads to tensor integrals  $P_{n_1, n_2}$  with  $n_1 \leq 4$  and  $n_2 < 4$ , or integrals with general  $(n_1, n_2)$  but with trivial numerators.

### C. Reduction of High-Multiplicity Integrals with Trivial Numerators

Once we have eliminated high-multiplicity tensor integrals, or equivalently those with non-trivial polynomials in  $\ell_{1,2}$  in the numerator, we must consider integrals with trivial numerators but arbitrary number of external legs. To reduce  $P_{n_1, n_2}$  integrals with  $n_1 \geq 5$ , we can make use of the same Gram determinant as in the one-loop case,

$$G\begin{pmatrix} \ell_1, 1, 2, 3, 4 \\ 5, 1, 2, 3, 4 \end{pmatrix} = 0. \quad (3.5)$$

We will obtain the reduction,

$$\begin{aligned} P_{n_1, n_2}(K_1, \dots, K_{n_1+n_2+2}) = & \\ & c_1 P_{n_1-1, n_2}(K_2, \dots, K_{(n_1+n_2+2)1}) + c_2 P_{n_1-1, n_2}(K_{12}, K_3, \dots, K_{n_1+n_2+2}) \\ & + c_3 P_{n_1-1, n_2}(K_1, K_{23}, K_4, \dots, K_{n_1+n_2+2}) + c_4 P_{n_1-1, n_2}(K_1, K_2, K_{34}, K_5, \dots, K_{n_1+n_2+2}) \\ & + c_5 P_{n_1-1, n_2}(K_1, \dots, K_{45}, \dots, K_{n_1+n_2+2}) + c_6 P_{n_1-1, n_2}(K_1, \dots, K_{56}, \dots, K_{n_1+n_2+2}), \end{aligned} \quad (3.6)$$

where the coefficients  $c_i$  are given in eq. (2.12), the same ones as in the one-loop reduction. This reduction involves only propagators dependent solely on  $\ell_1$ . (In the case  $n_1 = n_2$ ,  $P_{n_1-1, n_2}(\{K_i\}_1^{n_1}; \{K_j\}_{n_1+2}^{n_1+n_2+1})$  is given by the flipped integral  $P_{n_2, n_1-1}(\{K_j\}_{n_1+n_2+1}^{n_1+2}; \{K_i\}_{n_1}^1)$ .) This reduces the set of scalar integrals to  $P_{n_1, n_2}$  with  $n_2 \leq n_1 \leq 4$ . This means we have a finite (if large) set of integrals in terms of which we can express any planar two-loop integral, and hence any planar two-loop amplitude.

This reduction generalizes both to non-planar and to higher-loop integrals. The details are in some cases more intricate, but at two loops, we can reduce all integrals with more

than eleven propagators. We can see this using a variety of Gram determinant equations similar to eq. (3.5).

There is another, more general, way of looking at this question. Let us label the momenta in the two-loop vacuum diagram of fig. 3 by  $\ell_1$ ,  $\ell_2$ , and  $\ell_3$ . They are not independent, because  $\ell_1 + \ell_2 + \ell_3 = 0$ , but can be treated symmetrically. There can at most be eleven independent invariants  $t_i$  involving the loop momenta, namely the three squares of the loop momenta,

$$\ell_1^2, \quad \ell_2^2, \quad \ell_3^2; \quad (3.7)$$

and eight invariants built out of loop momenta, of the form

$$\ell_j \cdot k_i, \quad (3.8)$$

where four  $k_i$  are selected out of the external momenta. Because the external momenta are strictly four-dimensional, we can express all remaining ones, and hence all invariants involving them, in terms of these four. We can choose the invariants to be all manifestly reducible. If we have more than eight external lines attached to the lines in the vacuum diagram (that is, excluding legs attached directly to the vertices in it), then there are more than eleven propagators with denominators  $d_i$ , and accordingly we can write down non-trivial equations,

$$0 = d_i - \sum_j c_j t_j \quad (3.9)$$

for denominators beyond the eleventh. Inserting this equation into the integrand allows us to reduce the integrals with more than eleven propagators to simpler integrals, at arbitrary  $D$  or equivalently to all orders in  $\epsilon$ . (This assumes that the coefficient of the original integral is non-zero, which the earlier discussion demonstrates for the two-loop case.)

#### D. Integration-by-Parts Without Doubled Propagators

The reductions discussed in the previous subsections show that all required integrals for a planar  $n$ -point two-loop amplitude can be written in terms of the  $P_{4,4}$  integral with a trivial numerator;  $P_{4,n_2 < 4}$  integrals with trivial numerators or numerators dependent only on  $\ell_2$ ; and  $P_{n_1 < 4, n_2 \leq n_1}$  integrals with trivial numerators or numerators dependent on either or both of the loop momenta. Of course, some numerators can still be written as a difference of denominators, as in eq. (3.4). The corresponding integrals can then be reduced. The

remaining irreducible integrals, for  $n_1 + n_2 \geq 5$ , are those with irreducible numerators, which cannot be written in such a way. For example, in  $P_{4,3}$ ,  $\ell_2 \cdot K_1$  would be an irreducible numerator. (Some integrals with  $n_1 + n_2 \leq 4$  require a more specialized analysis, just as at one loop, and for the most part we shall not consider them in the present article.)

To reduce these integrals, where possible, we will employ the integration-by-parts (IBP) technique first introduced long ago by Chetyrkin and Tkachov [11], and refined into a general-purpose algorithm by Laporta [12].

The IBP technique as outlined by Laporta, and as implemented in **AIR** [13], **FIRE** [14], and **Reduze** [15], relies on writing down all possible equations from introducing a differentiation inside the integrand,

$$P_{n_1, n_2} \left[ \frac{\partial}{\partial \ell_j^\mu} v^\mu \right] = - \int \frac{d^D \ell_1}{(2\pi)^D} \frac{d^D \ell_2}{(2\pi)^D} \frac{\partial}{\partial \ell_j^\mu} \frac{v^\mu}{D(\ell_1, \ell_2, \{K_i\})} = 0, \quad (3.10)$$

where  $D(\ell_1, \ell_2, \{K_i\})$  is the denominator found in eq. (3.1). The simplest choices for  $v^\mu$  are the set of external momenta, along with the two loop momenta. The use of dimensional regularization ensures that there is no boundary term in this equation.

With these choices, however, the resulting equations involve not only the integrals of interest (as well as simpler planar integrals), but also integrals with doubled propagators. These arise from derivatives hitting the denominators of the integrals. Moreover, such integrals can have worse infrared singularities, so that their use results in the appearance of additional inverse powers of  $\epsilon$  in coefficients. This in turn would require them to be known (either analytically or numerically) to higher orders in  $\epsilon$ . These integrals do not arise directly in the computation of gauge-theory amplitudes, and usually we do not wish to introduce them at the stage of solving these equations. In all cases studied to date, it has been possible to eliminate such integrals (at a cost of retaining some integrals with non-trivial numerators), and it seems plausible that this holds true generally. Their elimination requires the consideration of very large systems of equations, performed using the Laporta algorithm. In addition to the considerable computational complexity of these systems, which has made it difficult to proceed in explicit examples beyond four-point integrals, it is also far from clear how to characterize these systems in the general case.

For this reason, we seek to simplify the equations we obtain by eliminating unwanted integrals, those with doubled propagators, from the very start. We will do so by making special choices of the  $v^\mu$  vectors in eq. (3.10). For example, we could choose vectors whose

dot product with the numerator resulting from differentiating any propagator vanishes,

$$v \cdot (\ell - K) = 0. \quad (3.11)$$

As these expressions are the coefficients of the doubled propagators, this vanishing will ensure that doubled propagators are absent. We can construct such vectors using Gram determinants; defining

$$G\left(\begin{matrix} \mu, b_1, b_2, b_3, b_4 \\ d_1, d_2, d_3, d_4, d_5 \end{matrix}\right) \equiv \frac{\partial}{\partial w_\mu} G\left(\begin{matrix} w, b_1, b_2, b_3, b_4 \\ d_1, d_2, d_3, d_4, d_5 \end{matrix}\right), \quad (3.12)$$

vectors  $v$  of the form

$$v^\mu = G\left(\begin{matrix} \mu, \ell_1, \ell_2, 6, 7, 8 \\ \ell_2, \ell_1, 1, 2, 3, 4 \end{matrix}\right) \quad (3.13)$$

will have the desired property with respect to propagators depending only on  $\ell_2$ . For example, the IBP equation,

$$P_{4,3}[\partial_2 \cdot v] = 0 \quad (3.14)$$

(where  $\partial_j = \partial/\partial\ell_j$ ), will be free of doubled propagators. Because  $\ell_{1,2}$  are  $D$ -dimensional vectors, Gram determinants like that in eq. (3.13) give the most general solution to eq. (3.11).

However, this solution is not general enough for our purposes. The problem is that while the constraint (3.11) is sufficient, it is not necessary. It is in general too strong a constraint, and in practice we would miss equations if we insisted on it. The weaker constraint, that

$$v \cdot (\ell - K) \propto (\ell - K)^2, \quad (3.15)$$

suffices to remove the doubled propagator as well. This constraint can be expressed as the requirement that there be no remainder upon synthetic division of  $v \cdot (\ell - K)$  by the propagator denominator  $(\ell - K)^2$ . We must impose this constraint for every propagator. For an integral with  $n_d$  propagators, that is with a denominator in the form,

$$W_n^{-1} \equiv \prod_{j=1}^{n_d} d_j = \prod_{j=1}^{n_d} (\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2, \quad (3.16)$$

we must impose the  $n_d$  equations

$$\text{Rem} \frac{[v_1 \cdot \frac{\partial}{\partial\ell_1} + v_2 \cdot \frac{\partial}{\partial\ell_2}](\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2}{(\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2} = 0, \quad (3.17)$$

or equivalently,

$$\text{Rem} \frac{[\sigma_{j1}v_1 + \sigma_{j2}v_2] \cdot (\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)}{(\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2} = 0, \quad (3.18)$$



where  $\text{Rem}$  denotes the remainder on synthetic division (using either  $\ell_i$  as a variable). (In these equations, the  $\sigma_j$  will be  $\pm 1$  or  $0$ .) These equations are for vectors  $v_{1,2}$  built out of the loop momenta, external momenta, and dot products thereof. We will discuss how to find the general solution to these equations in the next section. (By convention, we order the denominators as follows: first those depending only on the first loop momentum; then those depending only on the second loop momentum; and finally, those depending on both loop momenta.)

Before trying to solve the equations, let us try to characterize the solutions better. These have several general properties that will be helpful in finding and using these vectors. For example, if we have a pair of vectors,  $\{v_1^{(0)}, v_2^{(0)}\}$  that satisfy eq. (3.17), then any multiple of the pair is also a solution. In particular, multiplying by any Lorentz invariant involving either of the two loop momenta gives us a solution.

Not all these additional solutions are useful, however. We can divide these Lorentz invariants into two types: the reducible ones, expressible as a linear combination of propagator denominators and external invariants, and irreducible ones whose dependence on the loop momenta cannot be expressed using propagator denominators. While multiplying by an invariant of the former type does yield a solution to the constraints (3.17), it is not a useful solution, because it does not yield an independent equation for the integrals of irreducible numerators. To see this, let us write out the resulting IBP equations. The original equation is,

$$I[\partial_1 \cdot (v_1 W) + \partial_2 \cdot (v_2 W)] = 0. \quad (3.19)$$

Multiplying the vectors by a factor  $f$  gives a sum of two terms,

$$I[f(\partial_1 \cdot (v_1 W) + \partial_2 \cdot (v_2 W))] + I[W(v_1 \cdot \partial_1 f + v_2 \cdot \partial_2 f)] = 0. \quad (3.20)$$

The first term contains reduced integrals (that is, with fewer propagators) and terms proportional to the original equation. What about the second term? If  $f$  is reducible, its derivative can be written as a linear combination of the derivatives of the denominators in  $W$ . Because of eq. (3.18), the sum in parenthesis is strictly reducible, that is reducible *without* adding any terms proportional to external invariants. The second term in eq. (3.20) thus contributes only reduced integrals. Accordingly, only irreducible factors  $f$  can give rise to new IBP equations.

Indeed, the solution itself won't be useful if both of the vectors  $v_1$  and  $v_2$  are reducible; we will therefore restrict attention to solutions in which at least one is irreducible, that is, at least one term in one of the pair  $v_{1,2}$  is irreducible. Note that not all independent vectors will lead to independent IBP equations; but because the independence of the IBP equations can depend on whether the dimensional regulator  $\epsilon$  is taken to zero or not, we leave that assessment to a later stage.

It is possible to find even weaker constraints that remove double propagators, by adding a 'total derivative', that is a function which integrates to zero, to the right-hand side of eq. (3.15). We will not consider such right-hand sides. In the examples we consider below, they are not necessary, though we know of no general proof.

Integration-by-parts equations can be supplemented with Lorentz-invariance equations [34], using operators built out of derivatives with respect to external momenta. In general, these are not independent of the complete tower of IBP equations [42]; because we will be able to generate the complete tower of IBP equations, we do not need to consider Lorentz-invariance equations.

As mentioned in the introduction, for generalized unitarity, we only need to know the basis integrals, that is the set of integrals left independent by the full set of IBP equations. In order to find this set, we could of course solve for the IBP-generating vectors analytically, and then construct the set of IBP equations analytically as well. However, it suffices to solve for these vectors for a randomly-chosen ('generic') numerical configuration of external momenta. For higher-point integrals, or integrals with many massive external legs, this can greatly reduce the complexity of the calculation, and in particular the memory required to solve for the IBP-generating vectors.

### E. Additional Identities to $\mathcal{O}(\epsilon)$

The integration-by-parts identities give relations between different integrals that are valid for arbitrary dimension  $D$ , or equivalently, to all orders in the dimensional regulator  $\epsilon$ . However, in practical calculations at a given order in perturbation theory we are interested in computing terms only through  $\mathcal{O}(\epsilon^0)$ , and we are quite willing to drop terms of  $\mathcal{O}(\epsilon)$  or higher. Additional relations between integrals, even if they are only valid through  $\mathcal{O}(\epsilon^0)$ , are for these practical purposes just as good as relations that hold to all orders in  $\epsilon$ . The

reduction of the one-loop pentagon integral, as we reviewed in section II, is exactly this kind of relation. In general, we can write down several forms of integrands leading to integrals of  $\mathcal{O}(\epsilon)$ , built of Gram determinants or products thereof,

$$\begin{aligned} & G(\ell_1, b_1, b_2, b_3, b_4) G(\ell_2, b'_1, b'_2, b'_3, b'_4); \quad G\left(\begin{smallmatrix} \ell_1, b_1, b_2, b_3, b_4 \\ \ell_2, b'_1, b'_2, b'_3, b'_4 \end{smallmatrix}\right); \\ & G\left(\begin{smallmatrix} \ell_1, \ell_2, b_1, b_2, b_3 \\ \ell_1, \ell_2, b'_1, b'_2, b'_3 \end{smallmatrix}\right); \quad G\left(\begin{smallmatrix} \ell_1, \ell_2, b_1, b_2, b_3, b_4 \\ \ell_1, \ell_2, b'_1, b'_2, b'_3, b'_4 \end{smallmatrix}\right). \end{aligned} \quad (3.21)$$

where the momenta attached to the first loop (through which  $\ell_1$  flows) are contained either within the set  $\{b_1, b_2, b_3\}$  or within the set  $\{b'_1, b'_2, b'_3\}$ , and the momenta attached to the second loop are contained within the other of the two sets. These Gram determinants all vanish when either loop momentum approaches a potential (on-shell) collinear or soft configuration, thereby removing the corresponding divergences from the integral, and rendering it finite. In addition, the Gram determinants vanish when both loop momenta are four-dimensional, so that the integrals are of  $\mathcal{O}(\epsilon)$ . We can also write down differences of expressions yielding finite integrals which will again vanish when both loop momenta are four-dimensional, so that the resulting integrals are again of  $\mathcal{O}(\epsilon)$ ,

$$G\left(\begin{smallmatrix} \ell_1, b_1, b_2, b_3 \\ \ell_1, b_4, b_5, b_6 \end{smallmatrix}\right) G\left(\begin{smallmatrix} \ell_2, b'_1, b'_2, b'_3 \\ \ell_2, b'_4, b'_5, b'_6 \end{smallmatrix}\right) - G\left(\begin{smallmatrix} \ell_1, b_1, b_2, b_3 \\ \ell_2, b'_1, b'_2, b'_3 \end{smallmatrix}\right) G\left(\begin{smallmatrix} \ell_2, b'_4, b'_5, b'_6 \\ \ell_1, b_4, b_5, b_6 \end{smallmatrix}\right) \quad (3.22)$$

where the legs attached to the first loop are all represented amongst the  $b_i$ , and the legs attached to the second loop, amongst the  $b'_i$ . (For  $P^*$  and  $P^{**}$  integrals,  $k_1$  must also be amongst the  $b'_i$ , and  $k_n$  amongst the  $b_i$ ; for  $P^{**}$ ,  $k_{n+1}$  must be amongst the  $b_i$ , and  $k_{n+1}$  amongst the  $b'_i$ .)

Not all of these determinants will necessarily lead to useful equations reducing the basis. We can also consider integrals with numerators containing a product of one of these Gram determinants and other irreducible factors, so long as the integrals are ultraviolet-finite (which can be determined by power-counting). As is true for the IBP generating vectors, we can also generate additional identities for a randomly-chosen configuration of external momenta; this will be sufficient to identify the integrals that are independent through  $\mathcal{O}(\epsilon^0)$ . Typically, we will first solve all  $D$ -dimensional IBP equations, and use the solutions of those equations (in analytical or numerical form) to reduce the integrals obtained from inserting Gram determinants into the numerator; this will provide additional identities to  $\mathcal{O}(\epsilon^0)$  between the independent master integrals.

We can write down additional Gram determinants beyond those given in eq. (3.21),

$$G\left(\begin{smallmatrix} \ell_1, \ell_2, b_1, b_2, b_3 \\ \ell_1, b'_1, b'_2, b'_3, b'_4 \end{smallmatrix}\right); G\left(\begin{smallmatrix} \ell_1, \ell_2, b_1, b_2, b_3 \\ \ell_2, b'_1, b'_2, b'_3, b'_4 \end{smallmatrix}\right), \quad (3.23)$$

where all momenta attached to the second loop (with loop momentum  $\ell_2$ ) are represented amongst  $\{b_1, b_2, b_3\}$  in the first case, and similarly for the momenta attached to the first loop in the second case. However, these determinants give rise to integrands which are in fact total derivatives, and hence the corresponding integrals vanish identically. To see this, consider the following vector,

$$G\left(\begin{smallmatrix} \mu, \ell_1, \ell_2, b_1, b_2, b_3 \\ \ell_1, \ell_2, b'_1, b'_2, b'_3, b'_4 \end{smallmatrix}\right), \quad (3.24)$$

where all momenta attached to loop in which  $\ell_2$  flows are in  $\{b_{1,2,3}\}$ . The vector's dot product with the derivative of any propagator with respect to  $\ell_2$  will vanish so that only the derivative of the Gram determinant itself can enter any equation; but that derivative is proportional to the first determinant in eq. (3.23). Accordingly, we do not need to consider the forms in eq. (3.23) if we have already solved the IBP equations. If we include additional irreducible prefactors, we will again either obtain an expression proportional to the determinants in eq. (3.23) or to linear combinations of them and the last determinant in eq. (3.21). Equations similar to those considered in this section were obtained for six-point integrals by Cachazo, Spradlin, and Volovich [10] using leading singularities.

#### IV. IBP-GENERATING VECTORS

In order to find the general form of vectors leading to IBP equations free of doubled propagators, we must find the general solution to the set of equations (3.18). We begin by rewriting them in a somewhat more convenient form,

$$[\sigma_{j1}v_1 + \sigma_{j2}v_2] \cdot (\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j) + u_j (\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2 = 0, \quad (4.1)$$

where  $u_j$  is a polynomial in the various independent Lorentz invariants of the loop and external momenta. Because the different propagator denominators are independent (the integrals for which this is not true we have already treated in sects. IIIB and IIIC), this equation must hold for each of the  $n_d$  propagators independently.

Let us also write a general form for the  $v_i^\mu$ ,

$$v_i^\mu = c_i^{(\ell_1)}\ell_1^\mu + c_i^{(\ell_2)}\ell_2^\mu + \sum_{b \in B} c_i^{(b)}b^\mu, \quad (4.2)$$

where the sum runs over a set of  $n_B$  — up to four — basis vectors for the external momenta. (There would be four basis vectors for integrals with five or more external legs, and  $n - 1$  vectors for integrals with fewer.) Each of the coefficients  $c_i^{(x)}$  is again a polynomial in the various independent Lorentz invariants.

We consider as independent variables only invariants that are independent with respect to the loop momenta. That is,  $\ell_1^2$  and  $\ell_2^2$  are independent, as are each of these with respect to  $\ell_1 \cdot k_1$ , and a given invariant of the external momenta, say  $k_1 \cdot k_2$ . However, different invariants of external momenta are not independent, which is to say their ratio should be treated as a constant parameter. Let us pick the one independent invariant to be  $s_{12} = (k_1 + k_2)^2$ , and define the ratios,

$$\begin{aligned}\chi_{ij} &= \frac{s_{ij}}{s_{12}}, \\ \chi_{i\dots j} &= \frac{s_{i\dots j}}{s_{12}}, \\ \mu_i &= \frac{m_i^2}{s_{12}},\end{aligned}\tag{4.3}$$

in order to express the remaining invariants in terms of  $s_{12}$ . (For certain integrals with fewer than four external legs, we should pick a different invariant.) We will term these quantities parameters. Each of the coefficients  $c_i^{(x)}$  would have an expression in terms of the invariants,

$$V = \{\ell_1^2, \ell_1 \cdot \ell_2, \ell_2^2, \{\ell_1 \cdot b\}_{b \in B}, \{\ell_2 \cdot b\}_{b \in B}, s_{12}\}.\tag{4.4}$$

We treat these invariants as the basic symbols or variables out of which we build the solutions. For example, coefficients of engineering dimension two could be expressed as follows,

$$c_i^{(p)} = c_{i,1}^{(p)} s_{12} + \sum_{b \in B} c_{i,b1}^{(p)} \ell_1 \cdot b + \sum_{b \in B} c_{i,b2}^{(p)} \ell_2 \cdot b + c_{i,2}^{(p)} \ell_1^2 + c_{i,3}^{(p)} \ell_1 \cdot \ell_2 + c_{i,4}^{(p)} \ell_2^2.\tag{4.5}$$

The coefficients  $c_{i,j}^{(p)}$  of each term are rational functions of the parameters  $\chi_{i\dots j}$  and  $\mu_i$ . (In order to distinguish the different dimensions to which we will refer below, we refer to the engineering or energy dimension of  $\ell_i$  and  $b$  as such, dropping the ‘engineering’ qualifier only when context makes it unnecessary.)

Our discussion generalizes in a straightforward way both to higher loops and to non-planar integrals. At higher loops, we will have a vector  $v_l$  for each loop; the expansion (4.2) will have a sum over all loop momenta; and the set of variables  $V$  in eq. (4.4) will include all squares of loop momenta, all dot products of loop momenta with each other, and all dot

products of the loop momenta with the basis vectors in  $B$ . In general, some dot products of loop momenta with other loop momenta will be irreducible, but this does not change the derivation of the equations. For non-planar integrals at two loops, we will have more than a single equation involving two different vectors. (This will anyway be true at higher loops.) The general approach to solving the equations we now outline will also carry over, though the specific procedure that solves the equations most efficiently in these more general settings remains to be investigated. Internal masses will introduce additional parameters in eq. (4.3) while leaving the basic invariants (4.4) and the general structure unchanged.

Without loss of generality, we consider only solutions  $v_{1,2}$  of homogeneous engineering dimension. We could in principle proceed by writing down a general form for coefficients of a given engineering dimension, starting with dimension zero, and proceeding by increments of two. Plugging in these general forms into eq. (4.2), and requiring that the coefficient of each monomial in the basic variables (4.4) vanish independently, we would obtain the solutions of the given dimension.

This method of solution works quite well for finding solutions of low dimension, but becomes very memory-intensive for higher dimensions. Furthermore, it does not allow us to determine when we have found the complete independent basis set of solutions, namely the set of solutions  $v_{1,2}$  to eq. (4.2) in terms of which all others can be written as linear combinations, with coefficients that are polynomials in the basic variables (4.4) and rational in the parameters (4.3).

As a reminder, we are interested only in solutions for which at least one coefficient in either  $v_1$  or  $v_2$  is irreducible with respect to the set of denominators. Let us denote the operation of removing terms proportional to a propagator denominator (that is, reducing by the set of propagator denominators) by the operator  $\text{Irred}$ . It leaves behind only the irreducible part of an expression. (This operation is most naturally implemented using a Gröbner basis for the propagator denominators, but as these are all linear in the basic variables (4.4), the use of such a basis is not essential.) We defer a precise definition to later in this section.

We can assemble the set of equations eq. (4.1) into a single matrix equation. To do, first assemble the various coefficients using the relabeling,

$$\rho(\ell_1, 1) = 1,$$

$$\begin{aligned}
\rho(\ell_2, 1) &= 2, \\
\rho(j, 1) &= j + 2, \quad j \in \{1, \dots, n_B\}, \\
\rho(\ell_1, 2) &= n_B + 3, \\
\rho(\ell_2, 2) &= n_B + 4, \\
\rho(j, 2) &= n_B + j + 4, \quad j \in \{1, \dots, n_B\};
\end{aligned} \tag{4.6}$$

and the definitions,

$$\begin{aligned}
\tilde{c}_{\rho(q,i)} &= c_i^{(q)}, \quad q \in \{\ell_1, \ell_2\} \cup B, i \in \{1, 2\}, \\
\tilde{c}_{2n_B+4+j} &= u_j, \quad j \in \{1, \dots, n_d\}.
\end{aligned} \tag{4.7}$$

Treating the coefficients  $\tilde{c}$  as a row vector<sup>2</sup>, define

$$\begin{aligned}
E_{\rho(q,i),j} &= q \cdot \partial_i d_j, \\
E_{2n_B+4+j,j} &= -d_j.
\end{aligned} \tag{4.8}$$

$E$  is a  $(2n_B + 4 + n_d) \times n_d$ -dimensional matrix; the number of rows we will label  $n_r$ . Each column corresponds to eq. (4.1) for a different propagator. We then have the following matrix equation,

$$\tilde{c}E = 0. \tag{4.9}$$

Mathematicians call each solution to this equation a syzygy of  $E$ .

In intermediate stages, we may need to solve not only homogeneous equations such as this, but also inhomogeneous equations,

$$\tilde{c}E = f, \tag{4.10}$$

where the row vector  $f$  is independent of  $\tilde{c}$  though it may depend on other parameters.

Both of these equations are linear polynomial diophantine equations. In the adiatretoflu-ous language of mathematicians, the former is an equation for the syzygies of the ideal submodule of  $Q(\{\chi_{i\dots j}, \mu_i\})[V]^{n_d}$  generated by the rows of  $E$ ,

$$\text{Syz}(\langle \mathbf{e}_1, \dots, \mathbf{e}_n \rangle). \tag{4.11}$$

---

<sup>2</sup> Row vectors provide a more natural interpretation, as this choice also leads to treating the derivatives of the equation with respect to this vector's entries as row vectors, which in turn leads to a more natural implementation in a symbolic algebra language such as *Mathematica*.

More precisely, we seek a linearly-independent basis for the irreducible elements of the syzygy module,

$$\text{Syz}(\langle \mathbf{e}_1, \dots, \mathbf{e}_n \rangle) / \text{Syz}_{\text{Red}}(\langle \mathbf{e}_1, \dots, \mathbf{e}_n \rangle), \quad (4.12)$$

where the  $\text{Red}$  subscript denotes the reducible subspace with respect to Irred. In this language, it is basically a textbook problem, though there are aspects which require a bit more work than a textbook solution.

The solution relies on the use of Gröbner bases [43]. The reader may find an explanation of the varied uses of Gröbner bases, as well as algorithms for their construction, and the required background material, in several textbooks [44, 45]. Of these, we shall primarily make use of that Adams and Loustau [44]. Sturmfels gave a brief overview of Gröbner bases [46], and Lin et al. [47] also provide a nice introduction to Gröbner bases of modules from a physicist's point of view. Gröbner bases have been studied for use in integral reductions by Smirnov and Smirnov [48], and have been used by Smirnov in FIRE [14], as well as in other studies of integral reductions [49].

Our review here will mention only the minimal material needed for the description of the solution. Gröbner bases, amongst other uses, provide a certain generalization of linearly-independent bases to nonlinear multivariate polynomials. The basic setting is that of polynomials in a set of symbols. In our context, the symbols are those in the set  $V$  (4.4); the coefficients are arbitrary rational functions of the  $\chi_{i\dots j}$  and  $\mu_i$ , forming the field  $Q(\{\chi_{i\dots j}, \mu_i\})$  in mathematicians' language. We will need to consider vectors or tuples of polynomials as well as polynomials themselves.

The basic machinery requires us to choose an ordering of the terms built out of the basic symbols, as well as of tuples of terms. There are various ways of doing this, of which a lexicographic ordering is conceptually the simplest. While the choice of ordering will not change the space of solutions we find, the efficiency of the (standard) algorithms we employ *will* depend greatly on this choice. We choose the so-called degree-reverse lexicographic order (DRL or grevlex) for the basic symbols, and a term-over-position (ToP) ordering for tuples of polynomials. A generic term in a polynomial built out of the symbols  $x_i$  has the form,

$$c\mathbf{x}^{\mathbf{p}} \equiv cx_1^{p_1} \cdots x_n^{p_n}, \quad (4.13)$$



while a generic  $n$ -tuple of polynomials is a sum of terms of the form,

$$c\mathbf{v} \equiv c\mathbf{x}_v\mathbf{e}_v = cx_1^{p_1} \cdots x_n^{p_n} \mathbf{e}_v, \quad (4.14)$$

when the unit basis tuples are the set  $\{\mathbf{e}_j\}$ . The DRL ordering for polynomial terms starts with a basic ordering of the symbols  $x_n, \dots, x_1$  and orders  $\mathbf{x}^p$  before  $\mathbf{x}^q$  (denoted  $\mathbf{x}^p \prec \mathbf{x}^q$ ) iff,

$$\sum_i p_i < \sum_i q_i \quad \text{or} \quad \sum_i p_i = \sum_i q_i \text{ and the rightmost non-zero entry in } \mathbf{p} - \mathbf{q} \text{ is positive} \quad (4.15)$$

The ToP ordering orders tuples containing a lone monomial as follows,

$$\mathbf{v} \prec \mathbf{u} \Leftrightarrow \mathbf{x}_v \prec \mathbf{x}_u \quad \text{or} \quad \mathbf{x}_v = \mathbf{x}_u \text{ and } \mathbf{e}_v \prec \mathbf{e}_u. \quad (4.16)$$

(The basis vectors  $\mathbf{e}_j$  are ordered by their first non-zero component.) The *leading monomial* of a polynomial (or tuple)  $P$ , denoted  $\text{lm}(P)$ , is the monomial  $\mathbf{v}$  which is last in the ordering,  $\mathbf{v} \succ \mathbf{v}'$  for all monomials  $\mathbf{v}'$  in  $P$  (stripped of any coefficient  $c$ ).

With an ordering chosen, we can define a polynomial reduction algorithm, essentially a repeated synthetic division with respect to a basis set  $B$  of polynomials (or tuples), yielding a set of coefficients  $c$ , and a remainder  $r$ ,

$$p \xrightarrow{B} r, \quad (4.17)$$

where

$$p = \sum_{b \in B} c_b b + r. \quad (4.18)$$

The coefficients are again polynomials in the basic symbols, and the remainder is a polynomial (or tuple of polynomials if  $p$  is a tuple). At each stage of the synthetic division, a polynomial is divisible by a selected divisor iff its leading monomial is divisible by the divisor's leading monomial. For the purposes of synthetic division, we can treat  $n_d$ -dimensional tuples of polynomials by taking their dot product with an  $n_d$ -tuple of dummy or "tag" variables  $(t_1, \dots, t_{n_d})$ , and then performing ordinary synthetic division with the set of variables extended to include the tag variables  $t_i$ . The ToP/DRL ordering is then given by a DRL ordering, with the tag variables ordered before the other variables. One must ensure that other algorithms used maintain the linearity in these tag variables. At the end of a calculation, the tuples can be recovered by differentiating with respect to them.

In general, the reduction coefficients  $c_b$  in eq. (4.18) are not universally defined; they depend not only on the ordering chosen for monomials, but also on the order in which the polynomials are taken during synthetic division. Only if the set  $B$  of polynomials is a Gröbner basis will the reduction coefficients be independent of the order in which the polynomials are taken.

Let us write out the method of solution we have used, reverting to physicists' language, and postponing until the next section an explicit example, that of the massless double box. We use the Buchberger algorithm to compute the required Gröbner bases, though more sophisticated algorithms [50] are available and would be worth investigating. Using the algorithm, we compute the Gröbner basis of the set of rows of  $E$ , treated as  $n_d$ -tuples. We assemble the elements of the basis, again  $n_d$ -tuples, into a matrix  $G$ . The number of rows is determined by the number of tuples  $n_g$  in the Gröbner basis, which may be smaller, equal to, or larger than the number of original vectors  $n_r$  (which is equal to  $2n_B + n_d + 4$  in the case of  $E$ ). In addition to the basis itself, we will need the cofactor matrix  $C$ , which expresses the basis elements in terms of the original vectors,

$$G = CE. \quad (4.19)$$

It may be computed as a by-product of Buchberger's algorithm (or other algorithms) for computing the Gröbner basis. Because  $G$  is a Gröbner basis, we may also express each original vector as a linear combination of the basis vectors; this defines another matrix  $Q$ ,

$$E = QG. \quad (4.20)$$

In order to find the syzygies of  $E$ , we must first write down those of  $G$ . The syzygies of the latter — that is,  $n_g$ -tuples  $s$  such that  $sG = 0$  — can be constructed as described in the textbooks [44, 45]. The construction starts with the  $S$ -polynomial of two rows or basis  $n_d$ -tuples  $\mathbf{g}_{i,j}$ ,

$$S_p(\mathbf{g}_i, \mathbf{g}_j) = \frac{\text{lcm}(\text{lm}(\mathbf{g}_i), \text{lm}(\mathbf{g}_j))}{\text{lm}(\mathbf{g}_i)} \mathbf{g}_i - \frac{\text{lcm}(\text{lm}(\mathbf{g}_i), \text{lm}(\mathbf{g}_j))}{\text{lm}(\mathbf{g}_j)} \mathbf{g}_j, \quad (4.21)$$

where  $\text{lcm}$  denotes the least common multiple, with the added definition that  $\text{lcm}(\mathbf{e}_i, \mathbf{e}_j) \equiv 0$  if  $i \neq j$ . (The factors in front of  $\mathbf{g}_{i,j}$  are then pure polynomial terms, with the basis vectors  $\mathbf{e}$  canceling out.) The  $S$ -polynomial also plays a central role in the Buchberger algorithm itself. By construction, this  $S$ -polynomial can be completely reduced over the Gröbner basis,

$$S_p(\mathbf{g}_i, \mathbf{g}_j) = \sum_{k=1}^{n_g} h_k^{ij} \mathbf{g}_k; \quad (4.22)$$

Each syzygy or linear relation between the  $n_g$  Gröbner basis elements can be represented by an  $n_g$ -tuple, with basis elements  $\sigma_1, \dots, \sigma_{n_g}$ ,

$$\sigma_k G = g_k. \quad (4.23)$$

We can define a basic syzygy or linear relation,

$$\hat{s}_{ij} = \frac{\text{lcm}(\text{lm}(g_i), \text{lm}(g_j))}{\text{lm}(g_i)} \sigma_i - \frac{\text{lcm}(\text{lm}(g_i), \text{lm}(g_j))}{\text{lm}(g_j)} \sigma_j - \sum_{k=1}^{n_g} h_k^{ij} \sigma_k. \quad (4.24)$$

The complete set of syzygies of  $G$  is then generated by the set

$$\{\hat{s}_{ij} \mid 1 \leq i < j \leq n_g\}. \quad (4.25)$$

These syzygies, treated as row vectors, can again be assembled into a matrix  $S$ . With  $S$  in hand, the rows of  $SC$  are syzygies of  $E$ . In addition, because we must have

$$E = QG = QCE, \quad (4.26)$$

then  $(I - QC)E = 0$ , where  $I$  is the identity matrix. The rows of  $I - QC$  are thus also syzygies of  $E$ . We extend  $SC$  to add these rows. In our application, these turn out to be relevant only in some variants of the solution algorithms described below.

Not all syzygies, that is rows of  $S$ , are linearly independent. Indeed, there are typically dozens or even hundreds of syzygies. The set of syzygies can be reduced in a variety of ways, of which the two principal ones we use are polynomial reduction and numerically-assisted row reduction. Furthermore, as discussed earlier, we are interested only in rows of  $SC$  which are independent after reduction with respect to the propagator denominators, and this allows for additional reductions in number. For this purpose, we use the Irred operator described earlier. We define it as the polynomial reduction (element-by-element) with respect to a Gröbner basis  $G_D$  of the propagator denominators, built over the symbols in  $V$  (here using a plain lexicographic ordering),

$$p \xrightarrow{G_D} \text{Irred } p. \quad (4.27)$$

We apply polynomial reduction to the rows of  $S$ , treated as  $n_d$ -tuples, using a special ordering of the underlying variables, called the Schreyer ordering [44, 51]. It is defined by,

$$\mathbf{x}^p \mathbf{e}_i \prec \mathbf{y}^q \mathbf{e}_j \iff \text{lm}(\mathbf{x}^p \mathbf{g}_i) \prec \text{lm}(\mathbf{y}^q \mathbf{g}_j) \quad \text{or} \quad \text{lm}(\mathbf{x}^p \mathbf{g}_i) = \text{lm}(\mathbf{y}^q \mathbf{g}_j) \text{ and } j < i. \quad (4.28)$$

It is useful because the syzygy generators (4.25) form a Gröbner basis with respect to this ordering. When reducing syzygies, we start with those of lowest engineering dimension, removing those which reduce to zero (and hence are linear combinations of other syzygies), and proceed incrementally in the engineering dimension.

To find the set of fully-independent solutions modulo reducibility, we can proceed as follows to convert it to a linear algebra problem. We form the irreducible part of the solutions,

$$S^{\text{irred}} = \text{Irred } S, \quad (4.29)$$

and convert them into “tagged” polynomials using “tag” variables as described earlier. We now construct a vector space, in which each coordinate corresponds to a different monomial, and where each monomial that may appear in any of the tagged polynomials, or in any product of an irreducible polynomial times a tagged polynomial, is assigned a coordinate. Each tagged polynomial  $P$  (that is, each solution  $s$ ) may then be mapped to a vector  $\text{Vec}(s)$ , whose entries are rational functions of the  $\chi_{ij}$  and the  $\mu_i$ . Independence can then be determined by linear algebra (*e.g.* row reduction). We can check it numerically, by evaluating the solution for a given numerical choice of external momenta. For a given solution  $s$ , we also need to generate the vectors corresponding to multiples of  $s$  by a factor  $x$  built out of the variables in  $V$ . We can do this either by mapping the multiple,  $\text{Vec}(xs)$ , or by multiplying  $\text{Vec}(s)$  by the appropriate matrix. After removing linearly-dependent solutions, we usually end up with only a handful of independent syzygies, which we assemble into a matrix  $\overline{S}$ .

The general solution to eq. (4.9) can then be written as follows,

$$\tilde{c} = (p_1 \dots p_{n_s}) \overline{S}, \quad (4.30)$$

where  $n_s$  is the number of independent solutions, that is the rows of  $\overline{S}$ ; and where each  $p_i$  is an arbitrary polynomial in the variables in  $V$ . Because the Gröbner basis is finite, and of finite engineering dimension, the complete set of solutions is generated by a finite and finite-dimensional set, and any effectively reducible integral will be reduced by an IBP equation built using one of the basis elements (with a possible irreducible prefactor determined by the dimension of the numerator in the integral).

In order to solve inhomogeneous equations such as eq. (4.10), which will arise in some of the variants of the solution algorithm presented below, we must first reduce the right-hand

side  $f$  over the Gröbner basis of  $E$ ,

$$f = q_f G + r_f. \quad (4.31)$$

If  $r_f$  is non-vanishing, the equation has no solution. In our context,  $r_f$  will typically have one or more free coefficients  $p_i$  (arbitrary polynomials), and we will need to impose additional constraints on them to ensure that  $r_f$  becomes reducible over  $G$ . (It is not necessary to make it vanish strictly.) We can do so by solving the homogeneous equation,

$$r_f - \tilde{g}G = 0, \quad (4.32)$$

where  $\tilde{g}$  is an  $n_g$ -tuple of dummy coefficients. The solution will express the free coefficients  $p_i$  in  $r_f$  in terms of a more constrained set  $p'_i$ . The expression in terms of  $p'_i$  will now be reducible over  $G$ . Once we have solved this subsidiary equation (or if  $r_f$  vanishes to begin with), a particular solution to the inhomogeneous equation is given by

$$\tilde{c} = q_f C, \quad (4.33)$$

because then  $q_f C E = q_f G = f$ . In our solutions of inhomogeneous equations, we will not be interested in the general solution, but it can be obtained by adding an arbitrary solution to the corresponding homogeneous equation with  $f$  set to zero (obtained following the steps discussed above).

### A. A Simple Algorithm

The steps described in the previous section can be summarized in a simple algorithm (Algorithm I), which starts as input with a matrix  $E$  as in the form (4.9),

1. Compute the Gröbner basis  $G$  and the cofactor matrix  $C$  for the set of  $n_d$ -tuples given by the rows of  $E$ ;
2. Build the set of syzygies  $S$  of  $G$  using eq. (4.24);
3. Reduce the set of syzygies by synthetic division with respect to previous retained syzygies, discarding those with no remainder. It is best to proceed incrementally in the syzygies' engineering dimension;

4. Construct the matrix  $Q$  which expresses  $E$  in terms of  $G$ ;
5. Construct the set of solutions,  $SC$  along with  $I - QC$ ;
6. Reduce to a set of independent solutions with respect to reduction by the set of propagator denominators.

This algorithm works nicely and quickly for simple cases, such as the massless double box discussed in more detail in the next section. However, it suffers from very memory-intensive (and slow) intermediate stages for more complicated cases such as the four-mass double box or the pentabox, when the number of  $\chi$  and  $\mu$  parameters grows. There is room for improvement, because a great deal of unnecessary information (pertaining to fully-reducible solutions to the equations) is computed in intermediate stages.

## B. An Improved Algorithm

For these reasons, we use a somewhat more involved procedure. The greater complexity of the procedure is balanced by simpler execution at each stage. The basic idea is to split up the solution into several stages. We can split the matrix  $E$  and the desired coefficients  $\tilde{c}$  into reducible and irreducible parts,

$$\begin{aligned}
E^{\text{irred}} &= \text{Irred } E, \\
\tilde{c}^{\text{irred}} &= \text{Irred } \tilde{c}, \\
E^{\text{red}} &= E - E^{\text{irred}}, \\
\tilde{c}^{\text{red}} &= \tilde{c} - \tilde{c}^{\text{irred}}.
\end{aligned} \tag{4.34}$$

At the first stage, we solve the homogeneous set of irreducible equations,

$$\tilde{c}^{\text{irred}} E^{\text{irred}} = 0. \tag{4.35}$$

The full equation can then be rewritten as follows,

$$\tilde{c}^{\text{red}} E = -\tilde{c}^{\text{irred}} E^{\text{red}}, \tag{4.36}$$

which is an inhomogeneous equation for  $\tilde{c}^{\text{red}}$  in terms of the (now-known) irreducible polynomials  $\tilde{c}^{\text{irred}}$ . It turns out to be better to solve these equations in two stages, first only the

rows of  $E$  arising from propagators involving only  $\ell_1$  or  $\ell_2$ , but not both; and adding in the full set of equations in a second stage.

In order to solve the inhomogeneous equations, we write out an auxiliary set of equations which impose reducibility on each of the coefficients  $\tilde{c}^{\text{red}}$ ,

$$\tilde{c}_\alpha = \sum_{j=1}^{n_d} \tilde{c}_{\alpha,j} (\sigma_{j1}\ell_1 + \sigma_{j2}\ell_2 - K_j)^2. \quad (4.37)$$

The sum could also be taken over the Gröbner basis elements used to define the Irred operator. There are advantages and disadvantages to simply adding these equations as auxiliary equations, with additional unknowns  $\tilde{c}_{\alpha,j}$ , as opposed to substituting these expansions into the inhomogeneous equations (4.36), and both the memory usage and the time required for solving can depend sensitively on this choice. In the examples we have considered, it appears better not to substitute in the first of the two stages of solving the inhomogeneous equations, and better to substitute in the second stage.

At the first stage, we select the columns in eq. (4.36) corresponding to propagators involving either  $\ell_1$  or  $\ell_2$ , but not both; in the planar case, this means all but the last column. Call the solutions of these equations  $\tilde{c}_\alpha^{\text{II}}$ . At the second stage, we split the  $\tilde{c}_\alpha$ ,

$$\tilde{c}_\alpha = \tilde{c}_\alpha^{\text{II}} + \delta\tilde{c}_\alpha^{\text{red}}, \quad (4.38)$$

and solve eq. (4.36) for  $\delta\tilde{c}^{\text{red}}$ , with all but the last column of the right-hand side replaced by zero, and with an additional reducibility constraint of the form (4.37) imposed on  $\delta\tilde{c}^{\text{red}}$ .

The strategy for solving the inhomogeneous equations (4.10) can be summarized in the following algorithm (Algorithm II),

1. Compute the Gröbner basis  $G$  of the rows of  $E$  (it is sufficient to compute a partial Gröbner basis limited to the maximal engineering dimension found in the right-hand side  $f$ ), along with the cofactor matrix  $C$ ;
2. Reduce the right-hand side  $f$  over  $G$ , yield coefficients  $q_f$  and a remainder  $r_f$ ;
3. If the remainder  $r_f$  of this reduction does not vanish identically, solve the equation  $r_f - \tilde{g}G = 0$  with dummy coefficients  $\tilde{g}$  using Algorithm I (in practice, it is best to impose an engineering dimension limit in the intermediate steps of Algorithm I, and increment it until the solution converges to a stable one);

4. If a dimension-limited Gröbner basis was computed in step 1, and  $r_f$  was not identically zero at step 3, extend the Gröbner basis to the new (typically larger) maximal engineering dimension in the constrained form of  $f$ . Rather than starting from scratch, one can start from the original Gröbner basis  $G$ , in which case the full cofactor matrix will be given by the product of the new and old matrices,  $C_f = C_2 C_1$ .
5. The solution is then  $q_f C$ .

The improved strategy for solving the original equation (4.9) can then be summarized in the following algorithm (Algorithm III),

1. Compute solutions to eq. (4.35) using Algorithm I;
2. Solve the rows in the inhomogeneous equation (4.36) corresponding to propagators containing a lone loop momentum, for the reducible terms  $\tilde{c}^{\text{red}}$ , along with the constraint equations (4.37) expressing reducibility, using Algorithm II;
3. Write each coefficient  $\tilde{c}^{\text{red}}$  as a sum of this solution, and another coefficient  $\delta\tilde{c}^{\text{red}}$ , as in eq. (4.38). Solve the inhomogeneous equation corresponding to the propagator containing both loop momenta, along with constraint equations of step 2 with their right-hand sides set to zero, using Algorithm II (here it is better to substitute the reducibility constraint equations (4.37) back into the inhomogeneous equations);
4. Reduce to a set of independent solutions with respect to reduction by the set of propagator denominators.

## V. THE MASSLESS DOUBLE BOX

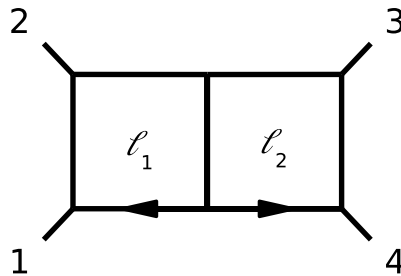


FIG. 5: The double box  $P_{2,2}^{**}$ .



As an example of how to apply the ideas presented in the previous section, let us examine the planar double box,  $P_{2,2}^{**}$ , with all external legs taken to be massless. The integral is shown in fig. 5. The  $D$ -dimensional reductions were worked out several years ago for the integral with all external masses vanishing, using AIR [13]. The same reductions have been worked out (though not reported explicitly) for configurations with one external mass [34]. The three- and four-mass cases have not been worked out previously. We discuss the massive cases in the next section.

As described in the previous section, we start by looking for vectors  $v_{1,2}^\mu$  that give rise to IBP equations free of doubled propagators. For the double box, we choose  $k_{1,2,4}$  as basis momenta, so the general form (4.2) becomes,

$$v_i^\mu = c_i^{(\ell_1)} \ell_1^\mu + c_i^{(\ell_2)} \ell_2^\mu + c_i^{(1)} k_1^\mu + c_i^{(2)} k_2^\mu + c_i^{(4)} k_4^\mu, \quad (5.1)$$

where each of the coefficients  $c^{(p)}$  is itself a function of Lorentz invariants in  $V$ , which here we can take to be the following set,

$$V_{22} = \{\ell_1^2, \ell_1 \cdot \ell_2, \ell_2^2, \ell_1 \cdot k_1, \ell_1 \cdot k_2, \ell_1 \cdot k_4, \ell_2 \cdot k_1, \ell_2 \cdot k_3, \ell_2 \cdot k_4, s_{12}\}. \quad (5.2)$$

The other dot products of the loop momenta can be expressed in terms of these via momentum conservation, and the other independent invariant is treated as a multiple of  $s_{12}$ ,  $s_{14} = \chi_{14} s_{12}$ . There are two irreducible numerators,  $\ell_1 \cdot k_4$  and  $\ell_2 \cdot k_1$ .

The matrix  $E$  of eq. (4.8) then takes the form,

$$E = 8 \begin{pmatrix} \ell_1^2 & -k_1 \cdot \ell_1 + \ell_1^2 & -k_1 \cdot \ell_1 - k_2 \cdot \ell_1 + \ell_1^2 & 0 \\ \ell_1 \cdot \ell_2 & -k_1 \cdot \ell_2 + \ell_1 \cdot \ell_2 & k_3 \cdot \ell_2 + k_4 \cdot \ell_2 + \ell_1 \cdot \ell_2 & 0 \\ k_1 \cdot \ell_1 & k_1 \cdot \ell_1 & k_1 \cdot \ell_1 - s_{12}/2 & 0 \\ k_2 \cdot \ell_1 & k_2 \cdot \ell_1 - s_{12}/2 & k_2 \cdot \ell_1 - s_{12}/2 & 0 \\ k_4 \cdot \ell_1 & k_4 \cdot \ell_1 - \chi_{14} s_{12}/2 & k_4 \cdot \ell_1 + s_{12}/2 & 0 \\ 0 & 0 & 0 & \ell_1 \cdot \ell_2 \\ 0 & 0 & 0 & \ell_2^2 \\ 0 & 0 & 0 & k_1 \cdot \ell_2 \\ 0 & 0 & 0 & -k_1 \cdot \ell_2 - k_3 \cdot \ell_2 - k_4 \cdot \ell_2 \\ 0 & 0 & 0 & k_4 \cdot \ell_2 \\ \ell_1^2/4 & 0 & 0 & 0 \\ 0 & \ell_1^2/4 - k_1 \cdot \ell_1/2 & 0 & 0 \\ 0 & 0 & \ell_1^2/4 + s_{12}/4 - k_1 \cdot \ell_1/2 - k_2 \cdot \ell_1/2 & 0 \\ 0 & 0 & 0 & \ell_2^2/4 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad (5.3)$$

$$\begin{pmatrix}
0 & 0 & \ell_1^2 + \ell_1 \cdot \ell_2 \\
0 & 0 & \ell_1 \cdot \ell_2 + \ell_2^2 \\
0 & 0 & k_1 \cdot \ell_1 + k_1 \cdot \ell_2 \\
0 & 0 & k_2 \cdot \ell_1 - k_1 \cdot \ell_2 - k_3 \cdot \ell_2 - k_4 \cdot \ell_2 \\
0 & 0 & k_4 \cdot \ell_1 + k_4 \cdot \ell_2 \\
-k_4 \cdot \ell_1 + \ell_1 \cdot \ell_2 & k_1 \cdot \ell_1 + k_2 \cdot \ell_1 + \ell_1 \cdot \ell_2 & \ell_1^2 + \ell_1 \cdot \ell_2 \\
-k_4 \cdot \ell_2 + \ell_2^2 & -k_3 \cdot \ell_2 - k_4 \cdot \ell_2 + \ell_2^2 & \ell_1 \cdot \ell_2 + \ell_2^2 \\
k_1 \cdot \ell_2 - \chi_{14} s_{12}/2 & k_1 \cdot \ell_2 + s_{12}/2 & k_1 \cdot \ell_1 + k_1 \cdot \ell_2 \\
(1 + \chi_{14}) s_{12}/2 - k_1 \cdot \ell_2 - k_3 \cdot \ell_2 - k_4 \cdot \ell_2 & s_{12}/2 - k_1 \cdot \ell_2 - k_3 \cdot \ell_2 - k_4 \cdot \ell_2 & k_2 \cdot \ell_1 - k_1 \cdot \ell_2 - k_3 \cdot \ell_2 - k_4 \cdot \ell_2 \\
k_4 \cdot \ell_2 & k_4 \cdot \ell_2 - s_{12}/2 & k_4 \cdot \ell_1 + k_4 \cdot \ell_2 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0 \\
-k_4 \cdot \ell_2/2 + \ell_2^2/4 & 0 & 0 \\
0 & \ell_2^2/4 + s_{12}/4 - k_3 \cdot \ell_2/2 - k_4 \cdot \ell_2/2 & 0 \\
0 & 0 & \ell_2^2/4 + \ell_1 \cdot \ell_2/2 + \ell_2^2/4
\end{pmatrix},$$

while the vector  $\tilde{c}$  is,

$$\tilde{c} = (c_1^{(\ell_1)} c_1^{(\ell_2)} c_1^{(1)} c_1^{(2)} c_1^{(4)} c_2^{(\ell_1)} c_2^{(\ell_2)} c_2^{(1)} c_2^{(2)} c_2^{(4)} u_{1\dots 7}). \quad (5.4)$$

The leftmost three columns correspond to equations for the left-hand loop; the following three columns, equations for the right-hand loop; and the last column, an equation for the common propagator.

The propagator denominators are,

$$\ell_1^2; (\ell_1 - k_1)^2; (\ell_1 - K_{12})^2; \ell_2^2; (\ell_2 - k_4)^2; (\ell_2 - K_{34})^2; (\ell_1 + \ell_2)^2. \quad (5.5)$$

Reducibility of an expression may be determined by reducing over a Gröbner basis of these denominators, which using a plain lexical ordering is,

$$\ell_1 \cdot \ell_2, \ell_2^2, k_4 \cdot \ell_2, k_3 \cdot \ell_2 - s_{12}/2, \ell_1^2, k_2 \cdot \ell_1 - s_{12}/2, k_1 \cdot \ell_1. \quad (5.6)$$

The Irred operator gives the remainder after this reduction; for example,

$$\begin{aligned}
& \text{Irred}(a_1 \ell_1^2 + a_2 \ell_1 \cdot \ell_2 + a_3 \ell_2^2 + a_4 \ell_1 \cdot k_1 + a_5 \ell_1 \cdot k_2 + a_6 \ell_1 \cdot k_4 + a_7 \ell_2 \cdot k_1 + a_8 \ell_2 \cdot k_3 \\
& \quad + a_9 \ell_2 \cdot k_4 + a_{10} s_{12}/2) \\
& = (a_5 + a_8 + a_{10}) s_{12}/2 + a_6 k_4 \cdot \ell_1 + a_7 k_1 \cdot \ell_2.
\end{aligned} \quad (5.7)$$

When using algorithm I from the previous section to solve eq. (4.9), we first obtain a Gröbner basis for the seven-tuples making up the rows of  $E$ . There are 50 tuples in this

basis, which in turn give rise to 167 syzygies, which we can represent as 17-tuples. Polynomial reduction and removal of completely-reducible syzygies (with respect to the basis in eq. (5.6)) leaves us with 119 syzygies of the Gröbner basis. These in turn give rise to 101 solutions of eq. (4.9), of which three are independent. The matrix  $I - QC$  gives no additional solutions (which can be understood on dimensional grounds here).

There is one solution whose coefficients are of engineering dimension two,

$$\begin{aligned} v_{1;1} &= -2(k_4 \cdot \ell_1 + \ell_1^2)k_1^\mu - \ell_1^2 k_2^\mu + (2k_1 \cdot \ell_1 - \ell_1^2)k_4^\mu + (4k_1 \cdot \ell_1 + 2k_2 \cdot \ell_1 + 2k_4 \cdot \ell_1 - s_{12})\ell_1^\mu, \\ v_{1;2} &= 2(\ell_2^2 - k_4 \cdot \ell_2)k_1^\mu + \ell_2^2 k_2^\mu + (2k_1 \cdot \ell_2 + \ell_2^2)k_4^\mu + (2k_3 \cdot \ell_2 - 2k_1 \cdot \ell_2 - s_{12})\ell_2^\mu; \end{aligned} \quad (5.8)$$

and two solutions with coefficients of engineering dimension four,

$$\begin{aligned} v_{2;1} &= (-4k_2 \cdot \ell_1 k_4 \cdot \ell_1 - 4k_3 \cdot \ell_2 \ell_1^2 + 4k_4 \cdot \ell_1 \ell_1^2 - 4k_4 \cdot \ell_2 \ell_1^2 - 4\ell_1^2 \ell_1 \cdot \ell_2 - 2\ell_1^2 \ell_2^2 - 2\chi_{14} \ell_1^2 s_{12})k_1^\mu \\ &\quad + (4k_1 \cdot \ell_1 k_4 \cdot \ell_1 - 2k_1 \cdot \ell_1 \ell_1^2 - 2k_2 \cdot \ell_1 \ell_1^2 - 4k_3 \cdot \ell_2 \ell_1^2 - 4k_4 \cdot \ell_2 \ell_1^2 - 4\ell_1^2 \ell_1 \cdot \ell_2 - 2\ell_1^2 \ell_2^2 \\ &\quad + 2\ell_1^2 s_{12} - 2\chi_{14} \ell_1^2 s_{12})k_2^\mu + (-4k_1 \cdot \ell_1 \ell_1^2 - 4k_2 \cdot \ell_1 \ell_1^2 + 2(\ell_1^2)^2 + 2\ell_1^2 s_{12})k_4^\mu \\ &\quad + (4k_1 \cdot \ell_1 k_2 \cdot \ell_1 + 4(k_2 \cdot \ell_1)^2 + 8k_1 \cdot \ell_1 k_3 \cdot \ell_2 + 8k_2 \cdot \ell_1 k_3 \cdot \ell_2 + 8k_2 \cdot \ell_1 k_4 \cdot \ell_1 + 8k_1 \cdot \ell_1 k_4 \cdot \ell_2 \\ &\quad + 8k_2 \cdot \ell_1 k_4 \cdot \ell_2 - 4k_4 \cdot \ell_1 \ell_1^2 + 8k_1 \cdot \ell_1 \ell_1 \cdot \ell_2 + 8k_2 \cdot \ell_1 \ell_1 \cdot \ell_2 + 4k_1 \cdot \ell_1 \ell_2^2 + 4k_2 \cdot \ell_1 \ell_2^2 \\ &\quad - 4k_1 \cdot \ell_1 s_{12} - 6k_2 \cdot \ell_1 s_{12} - 4k_3 \cdot \ell_2 s_{12} - 2k_4 \cdot \ell_1 s_{12} - 4k_4 \cdot \ell_2 s_{12} + \ell_1^2 s_{12} + 2\chi_{14} \ell_1^2 s_{12} \\ &\quad - 4\ell_1 \cdot \ell_2 s_{12} - 2\ell_2^2 s_{12} + 2s_{12}^2)\ell_1^\mu, \end{aligned} \quad (5.9)$$

$$\begin{aligned} v_{2;2} &= (4k_1 \cdot \ell_2 k_4 \cdot \ell_1 + 4k_3 \cdot \ell_2 k_4 \cdot \ell_1 + 4k_4 \cdot \ell_1 k_4 \cdot \ell_2 - 4k_4 \cdot \ell_2 \ell_1 \cdot \ell_2 + 4k_3 \cdot \ell_2 \ell_2^2 - 4k_4 \cdot \ell_1 \ell_2^2 \\ &\quad + 6\ell_1 \cdot \ell_2 \ell_2^2 + 4(\ell_2^2)^2 - 2\ell_1 \cdot \ell_2 s_{12} - 2\chi_{14} \ell_1 \cdot \ell_2 s_{12} - 2\ell_2^2 s_{12})k_1^\mu + (4k_1 \cdot \ell_2 k_4 \cdot \ell_1 \\ &\quad - 4k_4 \cdot \ell_2 \ell_1 \cdot \ell_2 + 2k_1 \cdot \ell_1 \ell_2^2 + 2k_2 \cdot \ell_1 \ell_2^2 + 4k_3 \cdot \ell_2 \ell_2^2 + 6\ell_1 \cdot \ell_2 \ell_2^2 + 4(\ell_2^2)^2 - 2\chi_{14} \ell_1 \cdot \ell_2 s_{12} \\ &\quad - 2\ell_2^2 s_{12})k_2^\mu + (4k_1 \cdot \ell_1 \ell_2^2 + 4k_2 \cdot \ell_1 \ell_2^2 + 4\ell_1 \cdot \ell_2 \ell_2^2 + 2(\ell_2^2)^2 - 2\ell_2^2 s_{12})k_4^\mu \\ &\quad + (-4k_3 \cdot \ell_2 k_4 \cdot \ell_2 - 4(k_4 \cdot \ell_2)^2 + 2k_3 \cdot \ell_2 \ell_2^2 + 2k_4 \cdot \ell_2 \ell_2^2 + 2k_1 \cdot \ell_2 s_{12} - 2\chi_{14} k_3 \cdot \ell_2 s_{12} \\ &\quad - 2\chi_{14} k_4 \cdot \ell_2 s_{12} + \ell_2^2 s_{12} + 2\chi_{14} \ell_2^2 s_{12})\ell_1^\mu + (4k_1 \cdot \ell_1 k_1 \cdot \ell_2 + 4k_1 \cdot \ell_2 k_2 \cdot \ell_1 + 4k_1 \cdot \ell_1 k_3 \cdot \ell_2 \\ &\quad + 4k_2 \cdot \ell_1 k_3 \cdot \ell_2 + 8(k_3 \cdot \ell_2)^2 + 8k_1 \cdot \ell_2 k_4 \cdot \ell_1 + 8k_3 \cdot \ell_2 k_4 \cdot \ell_2 + 8k_3 \cdot \ell_2 \ell_1 \cdot \ell_2 - 2k_1 \cdot \ell_1 \ell_2^2 \\ &\quad - 2k_2 \cdot \ell_1 \ell_2^2 + 8k_3 \cdot \ell_2 \ell_2^2 + 4k_4 \cdot \ell_2 \ell_2^2 - 2k_1 \cdot \ell_1 s_{12} - 2\chi_{14} k_1 \cdot \ell_1 s_{12} - 2k_2 \cdot \ell_1 s_{12} \\ &\quad - 2\chi_{14} k_2 \cdot \ell_1 s_{12} - 8k_3 \cdot \ell_2 s_{12} + 2k_4 \cdot \ell_1 s_{12} - 4k_4 \cdot \ell_2 s_{12} - 6\ell_1 \cdot \ell_2 s_{12} - 4\chi_{14} \ell_1 \cdot \ell_2 s_{12} \\ &\quad - 2\ell_2^2 s_{12} + 2s_{12}^2)\ell_2^\mu; \end{aligned}$$

and

$$v_{3;1} = (-4k_1 \cdot \ell_2 \ell_1^2 - \frac{2k_1 \cdot \ell_2 \ell_1^2}{\chi_{14}} - 2(\ell_1^2)^2 - \frac{(\ell_1^2)^2}{\chi_{14}} - 4\ell_1^2 \ell_1 \cdot \ell_2 - \frac{2\ell_1^2 \ell_1 \cdot \ell_2}{\chi_{14}} - 2k_2 \cdot \ell_1 \ell_2^2 - \frac{\ell_1^2 \ell_2^2}{\chi_{14}})$$

$$\begin{aligned}
& +\chi_{14}\ell_1^2s_{12} - 2\ell_1\cdot\ell_2s_{12} - 2\chi_{14}\ell_1\cdot\ell_2s_{12})k_1^\mu + (4k_1\cdot\ell_2k_4\cdot\ell_1 - 2k_1\cdot\ell_2\ell_1^2 - \frac{2k_1\cdot\ell_2\ell_1^2}{\chi_{14}} \\
& + 2k_3\cdot\ell_2\ell_1^2 + 2k_4\cdot\ell_2\ell_1^2 - 2(\ell_1^2)^2 - \frac{(\ell_1^2)^2}{\chi_{14}} - 4\ell_1^2\ell_1\cdot\ell_2 - \frac{2\ell_1^2\ell_1\cdot\ell_2}{\chi_{14}} + 2k_1\cdot\ell_1\ell_2^2 - 2\ell_1^2\ell_2^2 - \frac{\ell_1^2\ell_2^2}{\chi_{14}} \\
& + \chi_{14}\ell_1^2s_{12} - 2\chi_{14}\ell_1\cdot\ell_2s_{12})k_2^\mu + (-4k_1\cdot\ell_2k_2\cdot\ell_1 + 2k_1\cdot\ell_2\ell_1^2 + 2k_3\cdot\ell_2\ell_1^2 + 2k_4\cdot\ell_2\ell_1^2 \\
& + 2\ell_1\cdot\ell_2s_{12})k_4^\mu + (8k_1\cdot\ell_1k_1\cdot\ell_2 + \frac{4k_1\cdot\ell_1k_1\cdot\ell_2}{\chi_{14}} + 4k_1\cdot\ell_2k_2\cdot\ell_1 + \frac{4k_1\cdot\ell_2k_2\cdot\ell_1}{\chi_{14}} \\
& - 4k_2\cdot\ell_1k_3\cdot\ell_2 - 4k_1\cdot\ell_2k_4\cdot\ell_1 - 4k_3\cdot\ell_2k_4\cdot\ell_1 - 4k_2\cdot\ell_1k_4\cdot\ell_2 - 4k_4\cdot\ell_1k_4\cdot\ell_2 + 4k_1\cdot\ell_1\ell_1^2 \\
& + \frac{2k_1\cdot\ell_1\ell_1^2}{\chi_{14}} + 4k_2\cdot\ell_1\ell_1^2 + \frac{2k_2\cdot\ell_1\ell_1^2}{\chi_{14}} + 8k_1\cdot\ell_1\ell_1\cdot\ell_2 + \frac{4k_1\cdot\ell_1\ell_1\cdot\ell_2}{\chi_{14}} + 8k_2\cdot\ell_1\ell_1\cdot\ell_2 \\
& + \frac{4k_2\cdot\ell_1\ell_1\cdot\ell_2}{\chi_{14}} + \frac{2k_1\cdot\ell_1\ell_2^2}{\chi_{14}} + 4k_2\cdot\ell_1\ell_2^2 + \frac{2k_2\cdot\ell_1\ell_2^2}{\chi_{14}} - 2\chi_{14}k_1\cdot\ell_1s_{12} - 4k_1\cdot\ell_2s_{12} \\
& - \frac{2k_1\cdot\ell_2s_{12}}{\chi_{14}} - 2\chi_{14}k_2\cdot\ell_1s_{12} + 2k_3\cdot\ell_2s_{12} + 2\chi_{14}k_3\cdot\ell_2s_{12} + 2k_4\cdot\ell_2s_{12} + 2\chi_{14}k_4\cdot\ell_2s_{12} \\
& - 2\ell_1^2s_{12} - \frac{\ell_1^2s_{12}}{\chi_{14}} - \frac{2\ell_1\cdot\ell_2s_{12}}{\chi_{14}} + 4\chi_{14}\ell_1\cdot\ell_2s_{12} - \ell_2^2s_{12} - \frac{\ell_2^2s_{12}}{\chi_{14}} + \chi_{14}s_{12}^2)\ell_1^\mu + (2k_1\cdot\ell_1s_{12} \\
& + 2\chi_{14}k_1\cdot\ell_1s_{12} + 2\chi_{14}k_2\cdot\ell_1s_{12} - 2k_4\cdot\ell_1s_{12} - 2\ell_1^2s_{12} - 2\chi_{14}\ell_1^2s_{12})\ell_2^\mu, \tag{5.10} \\
v_{3;2} = & (-4k_4\cdot\ell_2\ell_1^2 - \frac{2k_4\cdot\ell_2\ell_1^2}{\chi_{14}} - 8k_4\cdot\ell_2\ell_1\cdot\ell_2 - \frac{4k_4\cdot\ell_2\ell_1\cdot\ell_2}{\chi_{14}} + 6k_1\cdot\ell_2\ell_2^2 + \frac{2k_1\cdot\ell_2\ell_2^2}{\chi_{14}} + 2k_3\cdot\ell_2\ell_2^2 \\
& - 2k_4\cdot\ell_2\ell_2^2 - \frac{2k_4\cdot\ell_2\ell_2^2}{\chi_{14}} + 4\ell_1^2\ell_2^2 + \frac{2\ell_1^2\ell_2^2}{\chi_{14}} + 8\ell_1\cdot\ell_2\ell_2^2 + \frac{4\ell_1\cdot\ell_2\ell_2^2}{\chi_{14}} + 2(\ell_2^2)^2 + \frac{2(\ell_2^2)^2}{\chi_{14}} \\
& - 2\ell_2^2s_{12} - 3\chi_{14}\ell_2^2s_{12})k_1^\mu + (4k_1\cdot\ell_2k_4\cdot\ell_2 + 4k_1\cdot\ell_2\ell_2^2 + \frac{2k_1\cdot\ell_2\ell_2^2}{\chi_{14}} - 2k_3\cdot\ell_2\ell_2^2 - 2k_4\cdot\ell_2\ell_2^2 \\
& + 2\ell_1^2\ell_2^2 + \frac{\ell_1^2\ell_2^2}{\chi_{14}} + 4\ell_1\cdot\ell_2\ell_2^2 + \frac{2\ell_1\cdot\ell_2\ell_2^2}{\chi_{14}} + 2(\ell_2^2)^2 + \frac{(\ell_2^2)^2}{\chi_{14}} - 3\chi_{14}\ell_2^2s_{12})k_2^\mu + (4(k_1\cdot\ell_2)^2 \\
& + 4k_1\cdot\ell_2k_3\cdot\ell_2 + 4k_1\cdot\ell_2k_4\cdot\ell_2 + 4k_1\cdot\ell_2\ell_1^2 + \frac{2k_1\cdot\ell_2\ell_1^2}{\chi_{14}} + 8k_1\cdot\ell_2\ell_1\cdot\ell_2 + \frac{4k_1\cdot\ell_2\ell_1\cdot\ell_2}{\chi_{14}} \\
& + 2k_1\cdot\ell_2\ell_2^2 + \frac{2k_1\cdot\ell_2\ell_2^2}{\chi_{14}} - 2k_3\cdot\ell_2\ell_2^2 - 2k_4\cdot\ell_2\ell_2^2 + 2\ell_1^2\ell_2^2 + \frac{\ell_1^2\ell_2^2}{\chi_{14}} + 4\ell_1\cdot\ell_2\ell_2^2 + \frac{2\ell_1\cdot\ell_2\ell_2^2}{\chi_{14}} \\
& + 2(\ell_2^2)^2 + \frac{(\ell_2^2)^2}{\chi_{14}} + 2\ell_2^2s_{12})k_4^\mu + (-4(k_1\cdot\ell_2)^2 + \frac{4k_1\cdot\ell_2k_3\cdot\ell_2}{\chi_{14}} - 4(k_3\cdot\ell_2)^2 + 4k_1\cdot\ell_2k_4\cdot\ell_2 \\
& + \frac{4k_1\cdot\ell_2k_4\cdot\ell_2}{\chi_{14}} - 4k_3\cdot\ell_2k_4\cdot\ell_2 - 4k_1\cdot\ell_2\ell_1^2 - \frac{2k_1\cdot\ell_2\ell_1^2}{\chi_{14}} + 4k_3\cdot\ell_2\ell_1^2 + \frac{2k_3\cdot\ell_2\ell_1^2}{\chi_{14}} \\
& - 8k_1\cdot\ell_2\ell_1\cdot\ell_2 - \frac{4k_1\cdot\ell_2\ell_1\cdot\ell_2}{\chi_{14}} + 8k_3\cdot\ell_2\ell_1\cdot\ell_2 + \frac{4k_3\cdot\ell_2\ell_1\cdot\ell_2}{\chi_{14}} - \frac{2k_1\cdot\ell_2\ell_2^2}{\chi_{14}} + 4k_3\cdot\ell_2\ell_2^2 \\
& + \frac{2k_3\cdot\ell_2\ell_2^2}{\chi_{14}} - 2k_1\cdot\ell_2s_{12} - \frac{2k_1\cdot\ell_2s_{12}}{\chi_{14}} + 2k_3\cdot\ell_2s_{12} - 2\chi_{14}k_3\cdot\ell_2s_{12} - 2\chi_{14}k_4\cdot\ell_2s_{12} \\
& - 2\ell_1^2s_{12} - \frac{\ell_1^2s_{12}}{\chi_{14}} - 4\ell_1\cdot\ell_2s_{12} - \frac{2\ell_1\cdot\ell_2s_{12}}{\chi_{14}} - 3\ell_2^2s_{12} - \frac{\ell_2^2s_{12}}{\chi_{14}} - 2\chi_{14}\ell_2^2s_{12} + \chi_{14}s_{12}^2)\ell_2^\mu.
\end{aligned}$$

The algorithms described in the previous section are not guaranteed to yield the solutions in the simplest possible form; it can happen that linear combinations of solutions can be

factored to yield a solution of lower engineering dimension. In this case, however, the solutions do appear to be close to the “simplest” possible ones.

Were we to use algorithm III, we would start by solving the equation for the irreducible part of  $E$ . Here, the Gröbner basis has 12 vectors, giving rise to five syzygies, and three solutions to eq. (4.35) — one with coefficients of engineering dimension two, the other two with coefficients of engineering dimension four. At the second stage, we have 103 basis tuples in the Gröbner basis (limited to engineering dimension six) for  $E$  augmented by the auxiliary equations (4.37) imposing reducibility. We find that the right-hand side of eq. (4.36) can be decomposed over this basis, so that  $r_f$  in eq. (4.31) vanishes. There are again three solutions to the equations. At the third stage, we include the last column of  $E$ , corresponding to the propagator involving both loop momenta; this yields 125 tuples in the Gröbner basis, and the right-hand side again reduces over this basis, and we end up with the three solutions prefigured by the solutions to the irreducible equations. In more complex integrals, the third stage will often impose additional constraints on the free polynomials obtained at the first stage, leading to fewer solutions, or more solutions with coefficients of higher engineering dimension.

The two algorithms are not guaranteed to produce the same solutions, and even for the massless double box, they do not. The solutions will however span the same space, and yield the same solutions to the IBP equations for the integrals of interest. In this case, they do produce the same number of solutions of each engineering dimension, and the solutions are equivalent — the solutions produced by algorithm I can be written as linear combinations of those produced by algorithm III and vice versa.

With the IBP generating vectors of eqns. (5.8) and (5.9), we can now construct IBP equations,

$$0 = P_{2,2}^{**} \left[ \frac{\partial}{\partial \ell_1^\mu} p v_{i;1}^\mu + \frac{\partial}{\partial \ell_2^\mu} p v_{i;2}^\mu \right], \quad (5.11)$$

where  $p$  is an irreducible polynomial in the symbols in  $V_{22}$ . These equations will relate various nominally-irreducible  $P_{2,2}^{**}$  to integrals with fewer propagators, but by construction will involve no undesired integrals. In practice, we do not need all three solutions; the first two suffice to produce all possible IBP equations.

The first solution (5.8) leads to the following equation,

$$0 = 2P_{2,2}^{**}[k_1 \cdot \ell_2](k_1, k_2, k_3, k_4) - 2P_{2,2}^{**}[k_4 \cdot \ell_1](k_1, k_2, k_3, k_4) + P_{2,1}^*[1](k_1, k_2, k_3, k_4) \quad (5.12)$$

$$-2P_{2,1}^*[1](k_3, k_4, k_1, k_2) + P_{2,1}^*[1](k_4, k_3, k_2, k_1) - P_{2,1}^{**}[1](k_1, k_2, K_{34}) + P_{2,1}^{**}[1](k_4, k_3, K_{12})$$

If we make use of the symmetries of the reduced integrals  $P_{2,1}^*$  and  $P_{2,1}^{**}$ , or reduce these latter integrals in turn, this equation simplifies to,

$$P_{2,2}^{**}[k_1 \cdot \ell_2](k_1, k_2, k_3, k_4) = P_{2,2}^{**}[k_4 \cdot \ell_1](k_1, k_2, k_3, k_4). \quad (5.13)$$

For the all-massless double box, this equation is also a direct consequence of the symmetries of the integral; but the analogous statement is no longer true for double boxes with external masses.

We can also use these vectors to derive equations for double boxes with more complicated numerator insertions, of powers or products of the basic irreducible numerators. As discussed earlier, we can do so by multiplying the vector by powers of invariants, which still yields a solution to the equations requiring that the IBP be free of doubled propagators.

In a gauge theory, 22 irreducible double boxes can arise:

$$\begin{aligned} &P_{2,2}^{**}[1], P_{2,2}^{**}[k_1 \cdot \ell_2], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2], P_{2,2}^{**}[(k_1 \cdot \ell_2)^3], P_{2,2}^{**}[k_4 \cdot \ell_1], \\ &P_{2,2}^{**}[(k_1 \cdot \ell_2)(k_4 \cdot \ell_1)], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2(k_4 \cdot \ell_1)], P_{2,2}^{**}[(k_1 \cdot \ell_2)^3(k_4 \cdot \ell_1)], P_{2,2}^{**}[(k_4 \cdot \ell_1)^2], \\ &P_{2,2}^{**}[(k_1 \cdot \ell_2)(k_4 \cdot \ell_1)^2], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2(k_4 \cdot \ell_1)^2], P_{2,2}^{**}[(k_1 \cdot \ell_2)^3(k_4 \cdot \ell_1)^2], P_{2,2}^{**}[(k_4 \cdot \ell_1)^3], \\ &P_{2,2}^{**}[(k_1 \cdot \ell_2)(k_4 \cdot \ell_1)^3], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2(k_4 \cdot \ell_1)^3], P_{2,2}^{**}[(k_1 \cdot \ell_2)^3(k_4 \cdot \ell_1)^3], P_{2,2}^{**}[(k_4 \cdot \ell_1)^4], \\ &P_{2,2}^{**}[(k_1 \cdot \ell_2)(k_4 \cdot \ell_1)^4], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2(k_4 \cdot \ell_1)^4], P_{2,2}^{**}[(k_1 \cdot \ell_2)^4], P_{2,2}^{**}[(k_1 \cdot \ell_2)^4(k_4 \cdot \ell_1)], \\ &P_{2,2}^{**}[(k_1 \cdot \ell_2)^4(k_4 \cdot \ell_1)^2], \end{aligned} \quad (5.14)$$

where we have omitted the momentum arguments  $k_1, k_2, k_3, k_4$  for brevity. In a gravitational theory, higher powers of the irreducible numerators may occur.

Two of the three IBP-generating vector pairs suffice to generate all possible IBP equations for these integrals (the third pair yields only linear combinations of the same equations). If we require that the coefficients be non-vanishing in the limit  $\epsilon \rightarrow 0$ , we find 19 equations; we can obtain an additional equation by relaxing this constraint. This allows us to eliminate 20 of the 22 integrals, solving for them in terms of integrals with fewer propagators and two irreducible master integrals, for example,

$$P_{2,2}^{**}[1] \text{ and } P_{2,2}^{**}[k_1 \cdot \ell_2]. \quad (5.15)$$

This reduction is the same as previously obtained with AIR [13] (and presumably by others). Even though the coefficients may be of order  $\epsilon$ , the solutions do *not* involve singular

coefficients for the double-box master integrals. (Because we do not fully reduce the simpler integrals, we cannot determine whether that is also true for them.) We do not need to study the full set of 22 integrals; a minimal set that reduces fully with the same two IBP-generating vectors is,

$$\{P_{2,2}^{**}[1], P_{2,2}^{**}[k_1 \cdot \ell_2], P_{2,2}^{**}[(k_1 \cdot \ell_2)^2], P_{2,2}^{**}[k_4 \cdot \ell_1], P_{2,2}^{**}[k_1 \cdot \ell_2 k_4 \cdot \ell_1], P_{2,2}^{**}[(k_4 \cdot \ell_1)^2]\} \quad (5.16)$$

In addition to the IBP equation (5.12) or (5.13), we have three additional equations for this set, arising from the first IBP-generating vector pair with prefactors  $k_4 \cdot \ell_1$  or  $k_2 \cdot \ell_2$ , and from the second IBP-generating vector pair with no prefactor.

The form of such minimal sets will in general depend on the dimensionality of the solution vectors; simplifying the IBP-generating vector pairs by taking linear combinations can in general lead to simpler minimal sets of effectively-reducible integrals.

The above reductions hold to all orders in the dimensional regulator  $\epsilon$ . We can also ask whether additional relations appear when we drop terms of  $\mathcal{O}(\epsilon)$  in the integrals. For the double box, there is only one Gram determinant which can lead to such a relation,

$$G(\ell_1, \ell_2, 1, 2, 4), \quad (5.17)$$

and one linear combination,

$$G(\ell_1, 1, 2, 4)G(\ell_2, 1, 2, 4) - G^2\left(\begin{smallmatrix} \ell_1, 1, 2, 4 \\ \ell_2, 1, 2, 4 \end{smallmatrix}\right). \quad (5.18)$$

When we use the IBP equations to reduce

$$P_{2,2}^{**}[G(\ell_1, \ell_2, 1, 2, 4)], \quad (5.19)$$

however, we find that the two irreducible master integrals (5.15) both appear with coefficients of  $\mathcal{O}(\epsilon)$ , and hence the Gram determinant fails to produce a useful relation. (More precisely, it provides only a relation for the divergent terms in the two integrals, but not for their finite terms.) The same is true for the combination of eq. (5.18). This strongly suggests that both integrals (5.15) that are independent to all orders in  $\epsilon$  remain linearly independent when truncated to  $\mathcal{O}(\epsilon^0)$ . (It doesn't provide a complete proof because we have not proven that the expressions (5.17) and (5.18) give all possible relations of this type.)

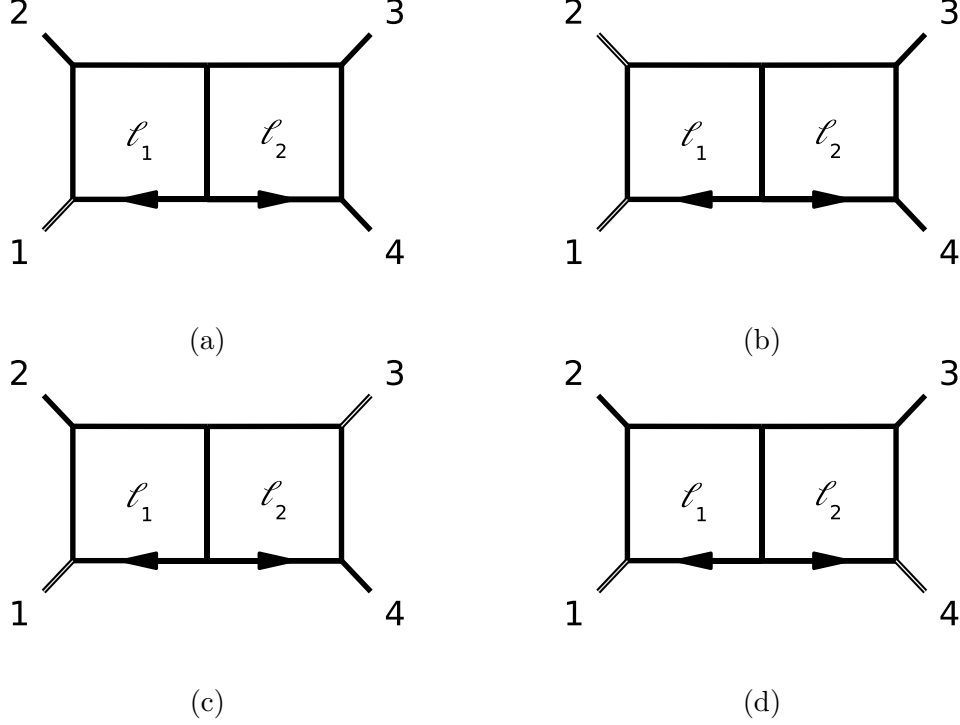


FIG. 6: Double boxes with external masses, with the massive legs indicated by doubled lines: (a) one-mass (b) short-side two-mass (c) diagonal two-mass (d) long-side two-mass.

## VI. MASSIVE DOUBLE BOXES

In this section, we survey the IBP-generating vectors for double boxes with some of the external legs taken to be massive. There is one possible configuration of masses if one external leg is massive, as is also true if three or four external legs are massive. With two massive external legs, there are three possible inequivalent integrals: both massive legs adjacent and attached to the same loop (‘short side’ or 2ms); the massive legs attached to diagonally-opposite corners (‘diagonal’ or 2md); or massive legs adjacent but attached to different loops (‘long side’ or 2ml). The one- and two-mass double boxes are shown in fig. 6.

We can use the same basis momenta and hence same form (5.1) and the same basic symbols (5.2) as in the massless case. Following the procedure outlined in section IV, we find three IBP generating vectors for the one-mass double box (we take leg 1 to be the massive one), once again one with coefficients of engineering dimension two, and two with coefficients of engineering dimension four. It again suffices to use the first two vectors to generate all possible IBP equations; there are again 20 equations for the 22 nominally-



irreducible integrals, giving rise to two irreducible master integrals, say,

$$P_{2,2}^{**}[1] \text{ and } P_{2,2}^{**}[k_1 \cdot \ell_2]. \quad (6.1)$$

The set of integrals in eq. (5.16) is again a minimal set that can be reduced. We will not display the IBP-generating vectors explicitly, but they are given in a companion *Mathematica* file.

For the long-side two-mass double box, we take legs 1 and 4 to be massive, and now find five IBP generating vectors, all with coefficients of engineering dimension four. There are again 20 equations for the 22 nominally-irreducible integrals, which we can derive using three of the five pairs of vectors. We can again pick the integrals in eq. (6.1) as irreducible masters.

For the diagonal two-mass double box, we take legs 1 and 3 to be massive, and use algorithm III to find three IBP generating vectors, with the same dimensions as the massless and one-mass cases. Once again, we need to use only two vector pairs to generate all required equations, and can take the integrals in eq. (6.1) as irreducible masters.

When we examine the short-side two-mass double box (taking legs 1 and 2 to be massive), we find our first surprise. Here we find four IBP generating vectors, all of engineering dimension four; but we find only 19 equations for the 22 original integrals (for which we need three of the four vector pairs), leaving us with three irreducible master integrals,

$$P_{2,2}^{**}[1], P_{2,2}^{**}[k_1 \cdot \ell_2], \text{ and } P_{2,2}^{**}[k_4 \cdot \ell_1]. \quad (6.2)$$

The three- and four-mass double boxes lead to very complicated analytic expressions in intermediate stages; it is much faster (and sufficient for the unitarity approach, as discussed earlier), to compute the IBP-generating vectors for a fixed numerical configuration of external momenta. We have chosen to do so; we find five IBP-generating vectors for the three-mass case (three with coefficients of dimension four, and two with coefficients of dimension six), and four vector pairs for the four-mass case (two each of dimensions four and six). In line with the result for the short-side two-mass double box, we find three master integrals for the three-mass case (which we can take to be those in eq. (6.2)). For the four-mass case, we find that we need four master integrals, which we can take to be,

$$P_{2,2}^{**}[1], P_{2,2}^{**}[k_1 \cdot \ell_2], P_{2,2}^{**}[k_4 \cdot \ell_1], \text{ and } P_{2,2}^{**}[k_1 \cdot \ell_2 k_4 \cdot \ell_1]. \quad (6.3)$$

In all cases, there are no additional equations that arise from truncation to  $\mathcal{O}(\epsilon)$ .

## VII. THE PENTABOX

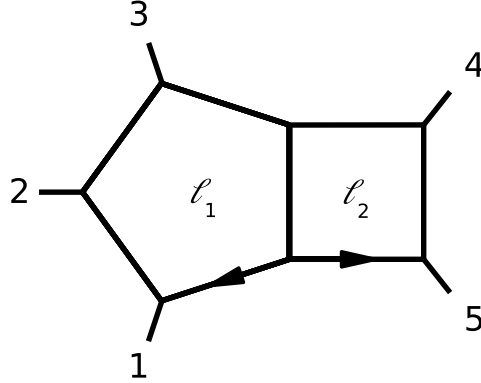


FIG. 7: The pentabox  $P_{3,2}^{**}$ .

Our next example is one of the three basic topologies that arise in five-point computations: the pentabox  $P_{3,2}^{**}$ , shown in fig. 7. Here, we choose  $k_{1,2,3,5}$  as basis momenta, so the general form (4.2) becomes,

$$v_i^\mu = c_i^{(\ell_1)} \ell_1^\mu + c_i^{(\ell_2)} \ell_2^\mu + c_i^{(1)} k_1^\mu + c_i^{(2)} k_2^\mu + c_i^{(3)} k_3^\mu + c_i^{(5)} k_5^\mu, \quad (7.1)$$

where again each of the coefficients  $c^{(p)}$  is a function of Lorentz invariants in the set of symbols  $V_{32}$ ,

$$V_{32} = \{\ell_1^2, \ell_1 \cdot \ell_2, \ell_2^2, \ell_1 \cdot k_1, \ell_1 \cdot k_2, \ell_1 \cdot k_3, \ell_1 \cdot k_5, \ell_2 \cdot k_1, \ell_2 \cdot k_2, \ell_2 \cdot k_4, \ell_2 \cdot k_5, s_{12}\}. \quad (7.2)$$

For this integral, we have constructed vectors both analytically and numerically; the numerical construction is much less memory-consuming. In both cases, the algorithms yield six IBP-generating vectors with coefficients of engineering dimension four, and three vectors with coefficients of dimension six. Their forms are too lengthy to display in the text, but are provided in the companion *Mathematica* file. There are 76 nominally-irreducible integrals in a gauge theory, involving powers of the three irreducible numerators,

$$k_1 \cdot \ell_2, k_2 \cdot \ell_2, k_5 \cdot \ell_1. \quad (7.3)$$

It suffices to use the six vector pairs of dimension four to generate all possible equations for these integrals. We find 73 such equations, leaving us with three truly-irreducible master integrals, which we can choose to be,

$$P_{3,2}^{**}[1], P_{3,2}^{**}[k_1 \cdot \ell_2], P_{3,2}^{**}[k_5 \cdot \ell_1]. \quad (7.4)$$

Examples of these reduction equations are,

$$\begin{aligned}
P_{3,2}^{**}[k_2 \cdot \ell_2] &= -\frac{(\chi_{15} - 2\chi_{23} + \chi_{23}\chi_{34} + 2\chi_{45} + \chi_{15}\chi_{45} - \chi_{34}\chi_{45})s_{12}}{4(\chi_{15} - \chi_{23} + \chi_{45})}P_{3,2}^{**}[1] \\
&\quad - \frac{(1 + \chi_{15} - \chi_{23} - \chi_{34})}{\chi_{15} - \chi_{23} + \chi_{45}}P_{3,2}^{**}[k_1 \cdot \ell_2] + \text{simpler integrals}, \\
P_{3,2}^{**}[k_1 \cdot \ell_2 k_2 \cdot \ell_2] &= \chi_{15} \left( \frac{1 + \chi_{15} - \chi_{34} - \chi_{45} - \chi_{15}\chi_{45} + \chi_{23}\chi_{45} + \chi_{34}\chi_{45}}{8(1 - 2\epsilon)(1 - \chi_{34} - \chi_{45})} \right. \\
&\quad + \frac{\epsilon(1 + \chi_{15} - \chi_{23} - \chi_{34})}{8(1 - 2\epsilon)(\chi_{15} - \chi_{23} + \chi_{45})(1 - \chi_{34} - \chi_{45})} \\
&\quad \left. \times (\chi_{15}(1 - \chi_{45}) + (\chi_{45} - \chi_{23})(2 - \chi_{34} - 2\chi_{45})) \right) s_{12}^2 P_{3,2}^{**}[1] \\
&\quad + \left( \frac{\epsilon(\chi_{15} + 2\chi_{15}\chi_{23} - 2\chi_{23}^2 - \chi_{23}\chi_{34} - \chi_{15}\chi_{45} + 2\chi_{23}\chi_{45} + \chi_{34}\chi_{45})}{2(1 - 2\epsilon)(\chi_{15} - \chi_{23} + \chi_{45})} \right. \\
&\quad \left. - \frac{2 + 2\chi_{15} - 3\chi_{34} - \chi_{15}\chi_{34} + \chi_{34}^2 - 2\chi_{45} - 2\chi_{15}\chi_{45} + \chi_{23}\chi_{45} + 2\chi_{34}\chi_{45}}{2(1 - 2\epsilon)(1 - \chi_{34} - \chi_{45})} \right) \\
&\quad \times s_{12} P_{3,2}^{**}[k_1 \cdot \ell_2] \\
&\quad - \frac{(1 + 2\epsilon)(1 + \chi_{15} - \chi_{23} - \chi_{34})(1 + \chi_{23} - \chi_{45})}{4(1 - 2\epsilon)(1 - \chi_{34} - \chi_{45})} s_{12} P_{3,2}^{**}[k_5 \cdot \ell_1] \\
&\quad + \text{simpler integrals}. \tag{7.5}
\end{aligned}$$

These master integrals are independent when considered to all orders in  $\epsilon$ . Unlike the case of the double box, however, here we *can* find two linear relations between them, so long as we truncate at  $\mathcal{O}(\epsilon^0)$ . These two relations arise from considering the following two integrals,

$$P_{3,2}^{**}\left[G\left(\begin{smallmatrix} \ell_1, 1, 2, 3, 5 \\ \ell_2, 1, 2, 3, 5 \end{smallmatrix}\right)\right] \text{ and } P_{3,2}^{**}\left[k_5 \cdot \ell_1 G\left(\begin{smallmatrix} \ell_1, 1, 2, 3, 5 \\ \ell_2, 1, 2, 3, 5 \end{smallmatrix}\right)\right] \tag{7.6}$$

both of which are of  $\mathcal{O}(\epsilon)$ , as discussed in section III E. Setting the two to zero, and using the reductions obtained from integration by parts, we find two equations relating the masters in eq. (7.4). We can use these, for example, to eliminate the two integrals with non-trivial numerators in favor of  $P_{3,2}^{**}[1]$ ,

$$\begin{aligned}
P_{3,2}^{**}[k_5 \cdot \ell_1] &= \frac{\chi_{15}\chi_{34}\chi_{45}s_{12}}{-\chi_{15} + \chi_{23} - \chi_{23}\chi_{34} + \chi_{15}\chi_{45} + \chi_{34}\chi_{45}}P_{3,2}^{**}[1] + \text{simpler integrals} + \mathcal{O}(\epsilon), \\
P_{3,2}^{**}[k_1 \cdot \ell_2] &= \frac{\chi_{15}(\chi_{15}(1 - \chi_{45})^2 + \chi_{34}(1 - \chi_{45})\chi_{45} - \chi_{23}(1 - \chi_{45} - \chi_{34}(1 + \chi_{45})))}{4(1 - \chi_{34} - \chi_{45})(\chi_{15} - \chi_{23} + \chi_{23}\chi_{34} - \chi_{15}\chi_{45} - \chi_{34}\chi_{45})}s_{12}P_{3,2}^{**}[1] \\
&\quad + \text{simpler integrals} + \mathcal{O}(\epsilon). \tag{7.7}
\end{aligned}$$

The other Gram determinants of the form suggested in section III E do not yield independent equations, but could be used instead to obtain equivalent equations. The longer denominators in these expressions may develop poles at exceptional values of the kinematics; these

are presumably spurious and are softened by the behavior of the various integrals in those limits, but we have not checked this. (Other denominators vanish in non-adjacent collinear limits, for example  $1 - \chi_{34} - \chi_{45} \rightarrow 0$  in the collinear limit  $k_3 \parallel k_5$ ; these are presumably spurious as well.)

One may wonder whether the IBP equations are even required for reduction of the truncated integrals, given the seemingly-stronger equations arising from Gram determinants. However, this strength is illusory: if we use only Gram determinant equations (including the IBP-like ones built from Gram determinants of the form given in eq. (3.23)), we find only 24 equations for 29 of the 35 integrals with numerators of dimension eight or less. (The IBP-like determinants provide two of these equations.) This would leave five seemingly-irreducible integrals as masters; of course, using the IBP equations, we could then reduce all of these to the scalar integral  $P_{3,2}^{**}[1]$ . If we consider the complete set of 76 integrals, we see another problem with using Gram-determinant equations alone: 20 of the integrals (those with four powers of  $\ell_2$ ) are ultraviolet divergent, which prevents us from using these equations to simplify them. In addition, even amongst the ultraviolet-finite integrals, we are left with five master integrals (there are 51 equations in total that we could derive).

### VIII. A SIX-POINT EXAMPLE

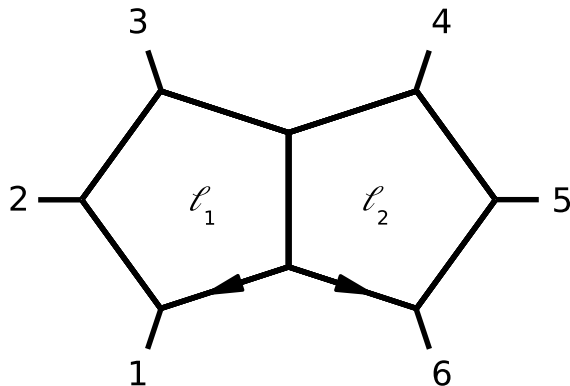


FIG. 8: The double pentagon  $P_{3,3}^{**}$ .

We will consider one example of a six-point integral, the so-called double pentagon  $P_{3,3}^{**}$ , shown in fig. 8. In contrast to the pentabox  $P_{3,2}^{**}$  considered in the previous section, we find that this integral can be reduced to simpler integrals entirely using Gram determinant

equations alone. Indeed, not only can integrals with non-trivial numerators be reduced, but the scalar integral itself,  $P_{3,3}^{**}[1]$ , can also be expressed in terms of simpler integrals (pentaboxes and products of one-loop pentagons, themselves reducible) via algebraic identities. We don't even need those Gram determinants equivalent to IBP equations to perform these reductions.

The double pentagon has two irreducible numerators, which we can pick to be  $k_6 \cdot \ell_1$  and  $k_1 \cdot \ell_2$ . There are thus 33 formally-irreducible integrals that arise in a gauge theory. The first thing to notice is that they are all ultraviolet-finite, so one of the obstructions that existed in the pentabox case to use of Gram-determinant equations alone for a complete reduction is absent here. There are 15 integrals of engineering dimension eight or less; exclude  $P_{3,3}^{**}[(k_6 \cdot \ell_1)^4]$  and  $P_{3,3}^{**}[(k_1 \cdot \ell_2)^4]$ , and examine the remaining 13 integrals. We can find 13 independent equations for them by starting with the following identities,

$$\mathcal{O}(\epsilon) = P_{3,3}^{**} \left[ p G \left( \begin{matrix} \ell_1, 1, 2, 3, 6 \\ \ell_2, 1, 2, 3, 6 \end{matrix} \right) \right], \quad (8.1)$$

with prefactors  $p = 1, k_1 \cdot \ell_2, (k_1 \cdot \ell_2)^2, k_6 \cdot \ell_1, (k_6 \cdot \ell_1)^2, k_1 \cdot \ell_2 k_6 \cdot \ell_1$ ;

$$\mathcal{O}(\epsilon) = P_{3,3}^{**} \left[ p G \left( \begin{matrix} \ell_1, \ell_2, 1, 2, 3 \\ \ell_1, \ell_2, 4, 5, 6 \end{matrix} \right) \right], \quad (8.2)$$

with prefactors  $p = 1, k_1 \cdot \ell_2, (k_1 \cdot \ell_2)^2, k_6 \cdot \ell_1, (k_6 \cdot \ell_1)^2$ ; and

$$\mathcal{O}(\epsilon) = P_{3,3}^{**} \left[ G \left( \begin{matrix} \ell_1, \ell_2, 1, 2, 4 \\ \ell_1, \ell_2, 3, 5, 6 \end{matrix} \right) \right] \quad \text{and} \quad \mathcal{O}(\epsilon) = P_{3,3}^{**} \left[ G \left( \begin{matrix} \ell_1, \ell_2, 1, 2, 5 \\ \ell_1, \ell_2, 3, 4, 6 \end{matrix} \right) \right]. \quad (8.3)$$

Similarly, if we examine the full set of 33 formally-irreducible integrals, we find 33 independent equations.

## IX. CONNECTION TO GENERALIZED UNITARITY

In this section, we use generalized unitarity to give a heuristic explanation for the structure of the results presented in previous sections. We begin, as in section II, with a discussion at one loop.

In basic unitarity at one loop, we examine the branch cut of amplitudes channel by channel. In each channel, the branch is a phase-space integral over a product of tree amplitudes. In the present paper, we are focused on loop integrals rather than complete amplitudes, so the equivalent statement — dating back to the Cutkosky rules [52] of the 1960s — is the

expression of the branch cut in terms of phase space integrals of scalar tree diagrams. The ordinary cut may be obtained by cutting two propagators, that is replacing the propagators by positive-energy delta functions which put the intermediate state on shell,

$$\frac{i}{(\ell - K)^2 + i\epsilon} \longrightarrow 2\pi\delta^{(+)}((\ell - K)^2). \quad (9.1)$$

(The (+) superscript indicates the restriction to positive energies.) There is nothing stopping us, however, from cutting more than two propagators, and this is the idea behind generalized unitarity. The solutions to the delta function constraints will in general then be complex, and so the delta functions must be understood in a more general sense, as contour integrals with the contours chosen to encircle the common solutions to the constraint equations. The idea of generalized unitarity was first applied as a practical tool for computation of amplitudes by Bern, Dixon, and one of the authors [23]. It was later combined with the use of complex momenta to give a general algebraic solution to finding the coefficients of box integrals [17], and used to derive a general and numerically-applicable technique for triangle and bubble integrals by Forde [19].

If one cuts as many propagators as possible, one arrives at maximal unitarity, as used for example in ref. [25, 53]. In old-fashioned language, this is equivalent to looking for ‘leading singularities’, discussed in a modern incarnation in ref. [54].

But how many propagators *can* we cut? If we examine a one-loop amplitude with all external momenta taken to be massive (so that infrared singularities are tamed), we can take the dimensional regulator  $\epsilon$  to zero, and perform the integrals in four dimensions. (Ignore the ultraviolet-divergent bubble in this discussion.) Each delta function will impose one constraint; because we have four components, we can have up to four delta functions. Attempting to impose additional delta functions will in general yield no solutions. (More precisely, because we will have more delta functions than integrals, the result will itself be a delta function rather than an ordinary function.) This in turn implies that functions with additional propagators may be determined in terms of functions with up to four propagators, as there are no additional degrees of freedom. In this case, all pentagons or higher-point integrals are reducible to sums of boxes and lower-point integrals.

The generalization of this observation to higher loops is straightforward. At each loop order, we have an additional four components. We can thus cut an additional four propagators. When considering infrared- and ultraviolet-finite integrals, then, we expect that only

those with up to four propagators per loop momentum will be algebraically independent. At two loops, this means that integrals with more than eight propagators, or more than four propagators involving a single loop momentum, will be reducible into simpler integrals.

Of course, the integrals of interest are in general infrared divergent. While the loop momentum is formally  $D$ -dimensional, so long as we keep the external momenta in four dimensions, the additional components  $\mu$  can only appear at one loop as  $\mu^2$ , on which we can impose one additional delta function. Thus when considering one-loop integrals to all orders in  $\epsilon$ , the pentagon integral must be taken as an additional independent integral, while higher-point integrals remain reducible. Now, the algebraic independence of the pentagon only manifests itself at  $\mathcal{O}(\epsilon)$ ; terms through  $\mathcal{O}(\epsilon^0)$  are reducible to sums of boxes. This reducibility is not manifest in our heuristic discussion; but it suggests the conjecture that the reducibility of integrals to  $\mathcal{O}(\epsilon^0)$  follows the pattern of massive reductions.

What happens at two loops? We now have two loop momenta, and correspondingly two  $\epsilon$ -dimensional vectors,  $\mu_1$  and  $\mu_2$ . These can now appear in integrals in the form of three independent quantities,  $\mu_1^2$ ,  $\mu_2^2$ , and  $\mu_1 \cdot \mu_2$ . We could impose additional delta functions on each, corresponding to cutting three additional propagators. For two-loop diagrams, we therefore expect any integral with more than eleven propagators, or more than five propagators involving a lone loop momentum, to be reducible to all orders in  $\epsilon$ . This is exactly what we found in section III.

Different propagators lead to different branch points (or branch surfaces, for the many-complex-variables functions we are considering). Accordingly, the algebraic independence of uncut propagators is clear. The algebraic independence of non-trivial numerators is less clear, as one might imagine algebraic relations between them. (Indeed, there are clearly algebraic relations between different powers of numerators, as seen in reduction equations elsewhere in the literature or in previous sections.) Heuristically, we do at least expect an upper bound,

$$\# \text{ irreducible non-trivial numerator integrals} \leq 11 - \# \text{propagators} . \quad (9.2)$$

This bound is respected by the explicit results in previous sections.

The question of algebraic independence when truncating integrals to  $\mathcal{O}(\epsilon)$  is more subtle. If we adopt the conjecture above suggested by one-loop results, it would imply that only truncated integrals with up to eight propagators (and up to four involving each loop

momentum) are algebraically independent. This is in agreement with the reducibility of the double-pentagon  $P_{3,3}^{**}$  discussed in section VIII. We might be further tempted to conjecture that the number of independent integrals with non-trivial numerators is limited to eight less the number of propagators. This would imply that there are no independent pentaboxes with irreducible numerators, which is in fact true. Thus the bound is respected by the pentabox results discussed in section VII, and also by the results for some double boxes; but it is violated for the short-side two-mass double box, as well as for double boxes with three or four external masses. The precise manner in which the heuristic picture breaks down remains to be clarified.

## X. CONCLUSIONS

Knowledge of an integral basis plays an important role in modern unitarity calculations. In this paper, we have given an outline of a basis for planar integrals (with massless propagators) at two loops. We distinguish two kinds of bases: the first, a set of integrals which are linearly independent to all orders in the dimensional regulator  $\epsilon$ ; the second, in which linear independence is required only through  $\mathcal{O}(\epsilon^0)$ .

Smirnov and Petukhov [29] have recently shown that the integral basis resulting from integration by parts is finite. We have delineated an explicit finite set of integrals which contains a minimal basis, and given an explicit procedure reducing an arbitrary planar two-loop gauge-theory integral to an element of this set. The set contains only integrals with four or fewer external legs attached to each line in the vacuum graph. All irreducible numerators, whose number depends on the external legs, are allowed in this finite set of integrals. The final basis contain only a subset of these integrals.

In order to reduce the set further, we then introduced an approach to generating integration-by-parts equations which involve only integrals in the desired set, along with simpler integrals (with propagators omitted), and avoiding integrals which are not ordinary Feynman integrals. For each of the integrals in the above set, one can solve for these vectors, and then determine the set of independent master integrals that make up the first,  $D$ -dimensional, basis. Unlike the situation at one loop, the reductions, and more importantly, the number of independent integrals, depend on the masses of the external legs. We gave a few examples of this type of calculation, but leave a complete study of the integrals



to future work.

We also introduced a special set of numerators, built using Gram determinants, which provide equations that yield identities for integrals truncated to  $\mathcal{O}(\epsilon^0)$ . These equations reduce the  $D$ -dimensional set of independent master integrals to a smaller set making up the second, “regulated four-dimensional” basis.

The general arguments as well as the notion of IBP-generating vectors and additional  $\mathcal{O}(\epsilon)$  identities generalize to non-planar integrals as well as to higher-loop integrals. We also expect them to generalize from the massless propagators considered here to integrals with massive propagators. It would also be interesting to explore the analog of the  $\mathcal{O}(\epsilon)$  identities for integrals in two- and three-dimensional field theories. We gave a heuristic argument for understanding the basis in terms of generalized unitarity; it would be interesting if it could be developed further to a complementary derivation for the reduction of integrals with formally-irreducible numerators to an independent set of master integrals.

The defining equations (4.9) for the IBP-generating vectors can also be thought of as defining a ‘surface’ or variety in the space whose coordinates are given by the different monomials in  $V$  (4.4). It would be interesting to explore its connection with the Grassmannians [55] introduced in recent explorations of integral coefficients in the  $\mathcal{N} = 4$  theory. The integral basis appropriate for the  $\mathcal{N} = 4$  theory should presumably make manifest (up to infrared divergences) its extended symmetries (conformal and dual conformal symmetries [37, 56]), and may make natural use of twistorial integrands such as those discussed in refs. [57].

Our approach to solving the required equations (4.1) for the IBP-generating made use of Gröbner bases, and in particular the standard Buchberger algorithm [43, 44] for computing them. The present implementation of the algorithm (coded in *Mathematica*) performs well for simple cases like the double box, but slows down and requires large memory in its intermediate stages for integrals with more legs or many massive legs. It would be worthwhile exploring the use of more modern algorithms, such as those of Faugère [50] for computing the required Gröbner bases.

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